



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 01:30 PM EST

PDB ID : 3J92  
EMDB ID : EMD-2832  
Title : Structure and assembly pathway of the ribosome quality control complex  
Authors : Shao, S.; Brown, A.; Santhanam, B.; Hegde, R.S.  
Deposited on : 2014-12-02  
Resolution : 3.60 Å(reported)  
Based on initial models : 4W20, 4W1Z

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

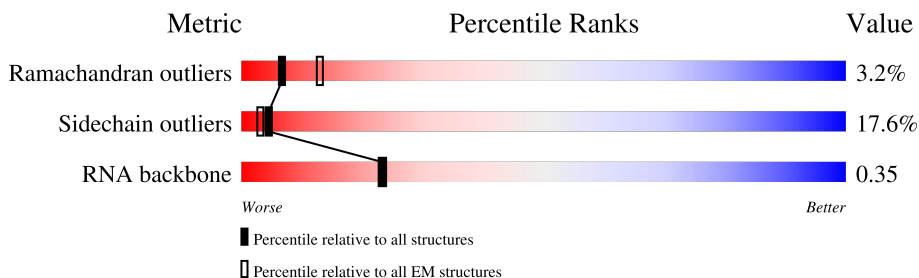
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



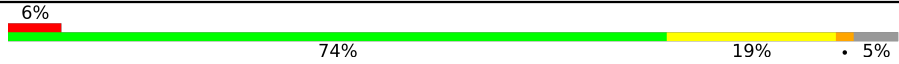
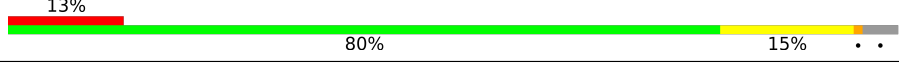
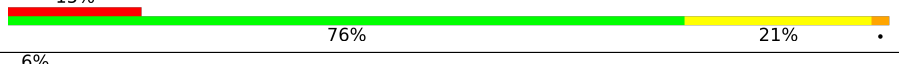


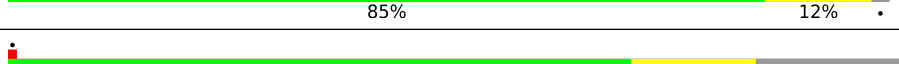
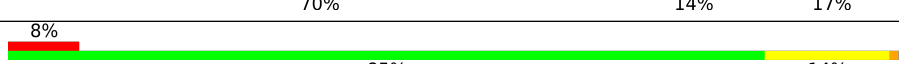
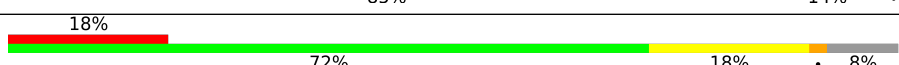
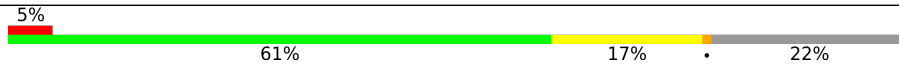


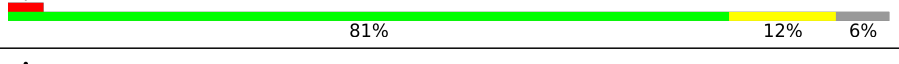


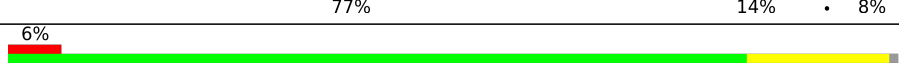

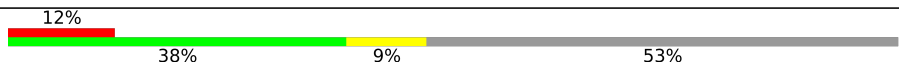








Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	
2	B	395	
3	C	368	
4	D	297	
5	E	284	
6	F	250	
7	G	266	
8	H	192	

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Mol	Chain	Length	Quality of chain
9	I	214	
10	J	178	
11	L	211	
12	M	213	
13	N	204	
14	O	204	
15	P	184	
16	Q	188	
17	R	196	
18	S	224	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	160	
28	c	115	
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	

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Mol	Chain	Length	Quality of chain
34	i	105	10% 81% 14% . .
35	j	97	. 69% 20% 11%
36	k	70	24% 74% 24% .
37	l	51	10% 76% 18% . .
38	m	128	. 30% 9% . 59%
39	o	106	10% 77% 18% . .
40	p	92	9% 82% 16% . .
41	r	137	9% 74% 16% . 9%
42	s	317	47% 52% 10% . 38%
43	t	165	78% 71% 25% . .
44	u	501	26% 24% . 74%
44	v	501	15% 23% . 73%
45	0	1766	. 98%
45	w	1766	. 99%
45	z	1766	. 6% . 93%
46	x	218	53% 100%
46	y	218	59% 97% .
47	1	104	5% 11% . . 86%
48	2	77	91% 55% 43% .
49	5	3664	10% 60% 37% .
50	7	120	. 76% 24%
51	8	156	6% 68% 31% .

## 2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 146386 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	244	1868	1171	382	309	6	0	0

- Molecule 2 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	394	3147	2005	591	538	13	0	0

- Molecule 3 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	367	2919	1836	582	486	15	0	0

- Molecule 4 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	292	2384	1511	435	426	12	0	0

- Molecule 5 is a protein called eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	236	1904	1219	364	316	5	0	0

- Molecule 6 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	225	1870	1202	358	301	9	0	0

- Molecule 7 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	241	1939	1235	372	328	4	0	0

- Molecule 8 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	190	1518	956	284	272	6	0	0

- Molecule 9 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	204	1651	1048	318	271	14	0	0

- Molecule 10 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	170	1359	856	256	241	6	0	0

- Molecule 11 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	210	1703	1064	354	280	5	0	0

- Molecule 12 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	138	1131	727	216	181	7	0	0

- Molecule 13 is a protein called eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	203	1701	1072	359	266	4	0	0

- Molecule 14 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	199	Total	C	N	O	S	0	0
			1638	1056	321	256	5		

- Molecule 15 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 16 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	187	Total	C	N	O	S	0	0
			1506	941	311	249	5		

- Molecule 17 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 18 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	175	Total	C	N	O	S	0	0
			1454	925	284	235	10		

- Molecule 19 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 20 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 21 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 22 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 23 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 24 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 25 is a protein called eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 26 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	147	Total	C	N	O	S	0	0
			1163	735	239	185	4		

- Molecule 27 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	75	Total	C	N	O	S	0	0
			610	378	130	99	3		

- Molecule 28 is a protein called eL30.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	94	732	465	130	131	6	0	0

- Molecule 29 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	107	888	560	171	155	2	0	0

- Molecule 30 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	128	1053	667	216	165	5	0	0

- Molecule 31 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	109	876	555	174	144	3	0	0

- Molecule 32 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	114	906	566	187	147	6	0	0

- Molecule 33 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	122	1015	642	205	167	1	0	0

- Molecule 34 is a protein called eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	102	832	521	177	129	5	0	0

- Molecule 35 is a protein called eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	86	Total	C	N	O	S	0	0
			706	436	155	110	5		

- Molecule 36 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 38 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 39 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 40 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 41 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	125	Total	C	N	O	S	0	0
			1001	622	206	168	5		

- Molecule 42 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	s	198	Total	C	N	O	S	0	0
			1522	968	265	280	9		

- Molecule 43 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	t	163	Total	C	N	O	S	0	0
			1238	773	230	230	5		

- Molecule 44 is a protein called NEMF.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	u	130	Total	C	N	O		0	0
			645	385	130	130			
44	v	136	Total	C	N	O	S	0	0
			1092	687	197	206	2		

- Molecule 45 is a protein called Listerin.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	w	15	Total	C	N	O		0	0
			110	67	23	20			
45	z	130	Total	C	N	O	S	0	0
			1057	681	180	189	7		
45	0	36	Total	C	N	O	S	0	0
			293	187	53	48	5		

- Molecule 46 is a protein called Listerin.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	x	218	Total	C	N	O	0	0
			1090	654	218	218		
46	y	211	Total	C	N	O	0	0
			1055	633	211	211		

- Molecule 47 is a protein called nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1	15	Total	C	N	O	S	0	0
			125	82	20	22	1		

- Molecule 48 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
48	2	75	1601	715	292	520	74	0	0

- Molecule 49 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
49	5	3662	78486	34947	14363	25515	3661	0	0

- Molecule 50 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	7	120	2558	1141	456	842	119	0	0

- Molecule 51 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	8	156	3314	1480	585	1094	155	0	0

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	P	1	Total	Mg	0
			1	1	
52	V	1	Total	Mg	0
			1	1	
52	g	1	Total	Mg	0
			1	1	
52	5	150	Total	Mg	0
			150	150	
52	7	5	Total	Mg	0
			5	5	
52	8	1	Total	Mg	0
			1	1	

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	g	1	Total	Zn	0
			1	1	

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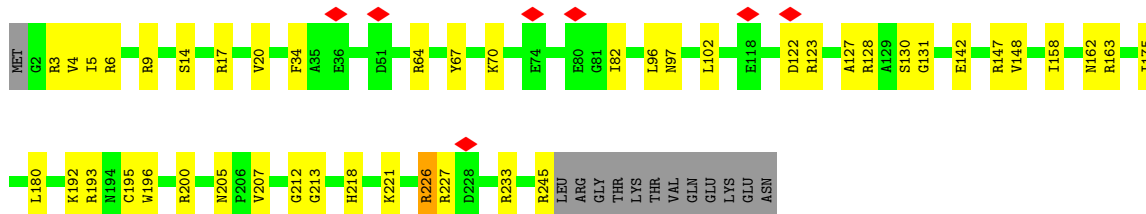
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53	j	1	Total 1	Zn 1	0
53	m	1	Total 1	Zn 1	0
53	o	1	Total 1	Zn 1	0
53	p	1	Total 1	Zn 1	0

### 3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

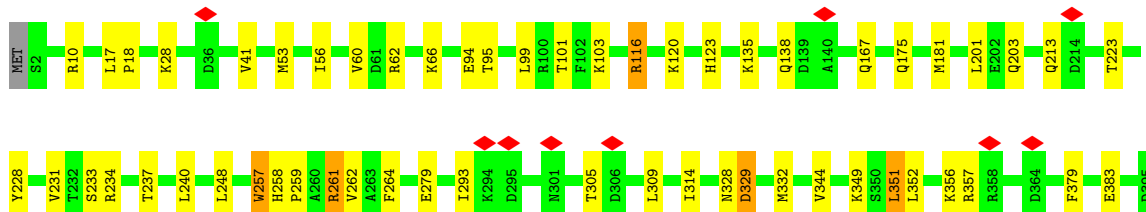
- Molecule 1: uL2

Chain A: 




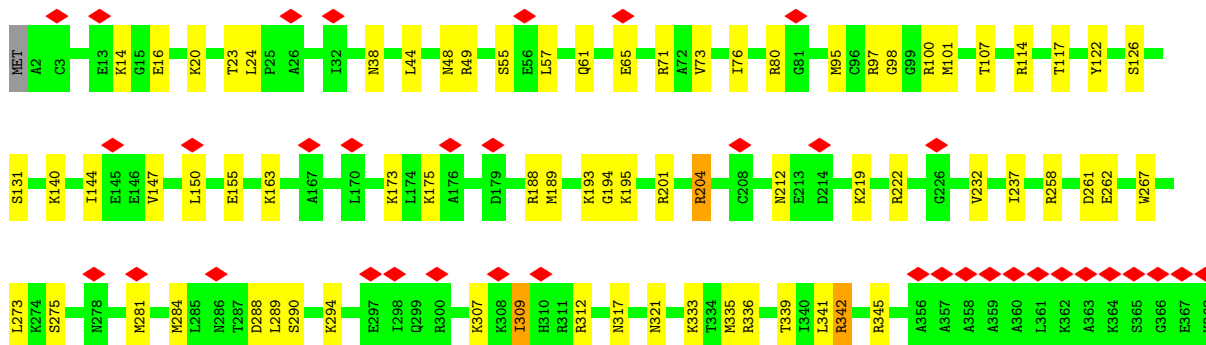
- Molecule 2: uL3

Chain B: 



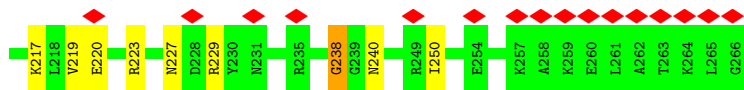
- Molecule 3: uL4

Chain C: 

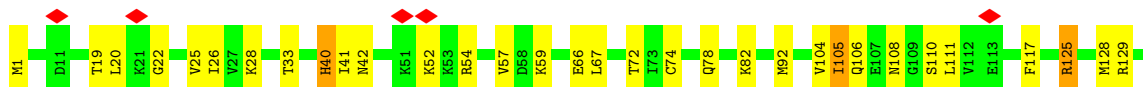
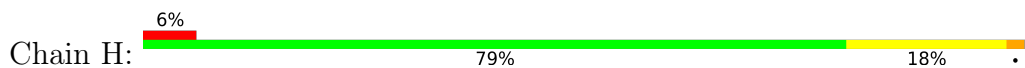


- Molecule 4: uL18





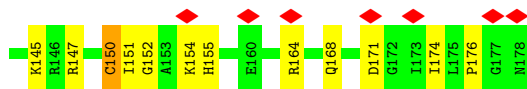
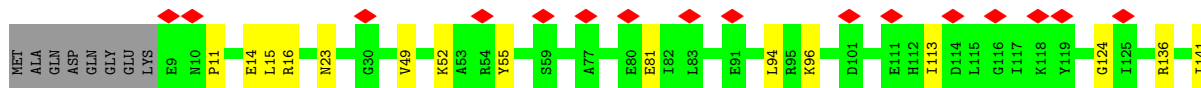
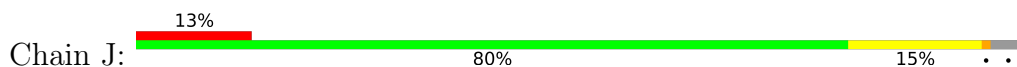
• Molecule 8: uL6



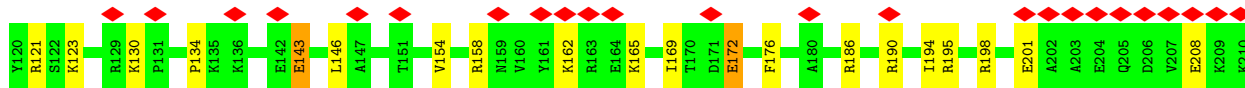
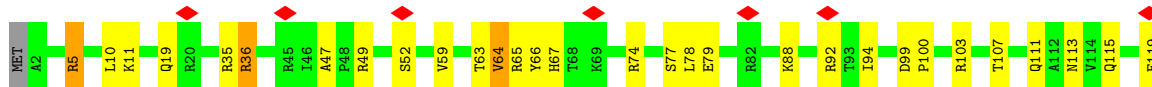
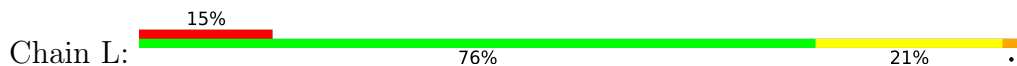
• Molecule 9: uL16



• Molecule 10: uL5



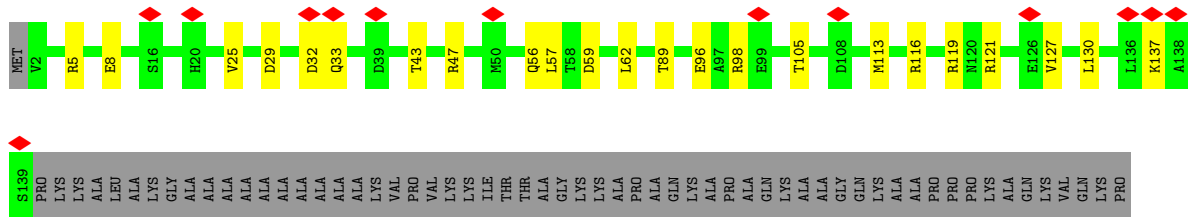
• Molecule 11: eL13





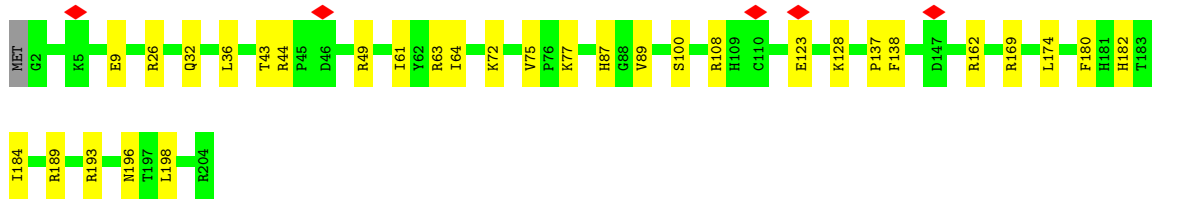
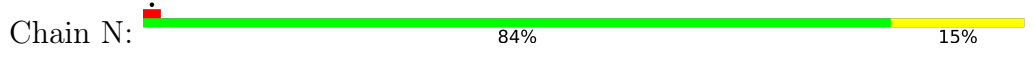
K211

• Molecule 12: eL14

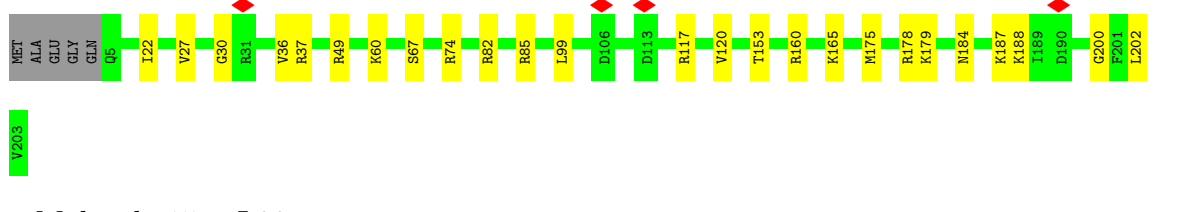
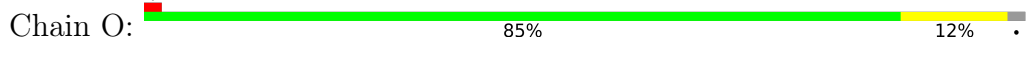


PRO  
ALA  
GLN  
LYS  
LYS  
ALA  
LEU  
ALA  
ALA  
PRO  
LYS  
GLY  
ALA  
SER  
GLY  
GLU  
LYS  
ALA

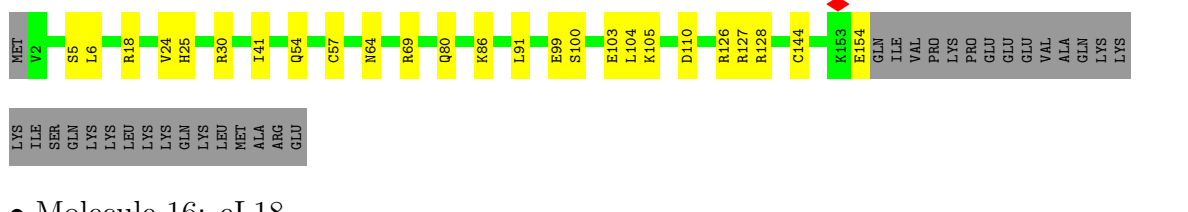
• Molecule 13: eL15



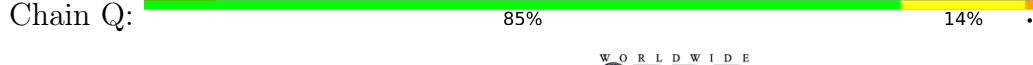
• Molecule 14: uL13

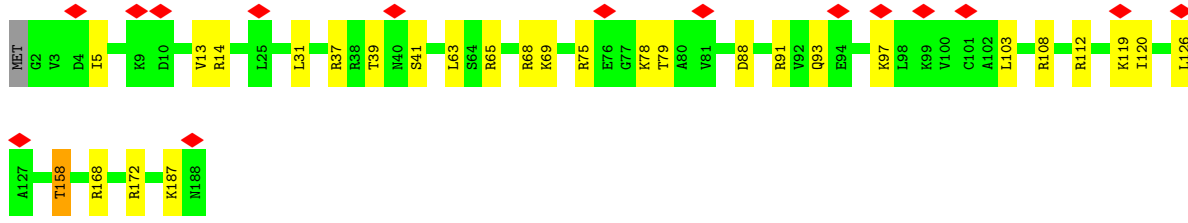


• Molecule 15: uL22

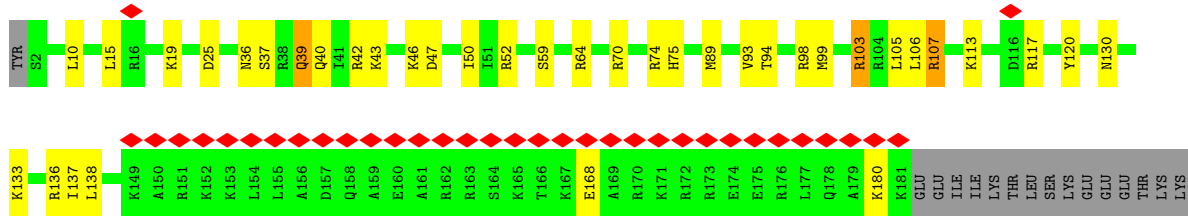
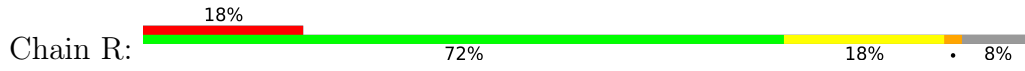


• Molecule 16: eL18

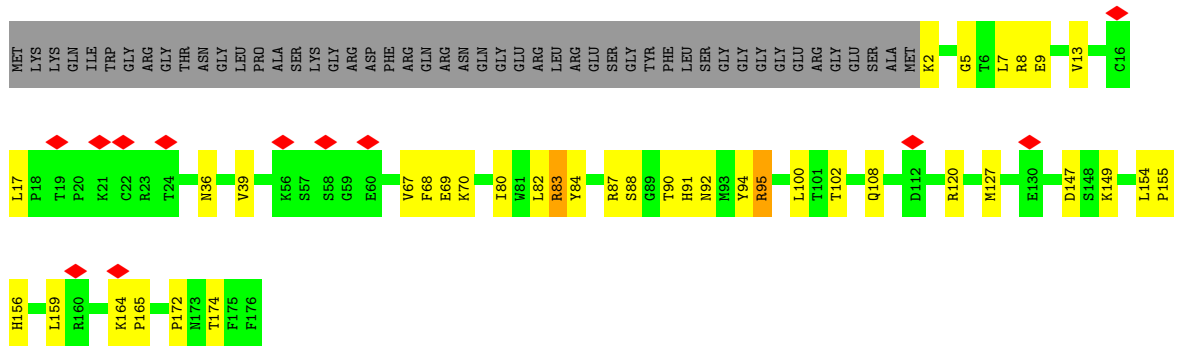




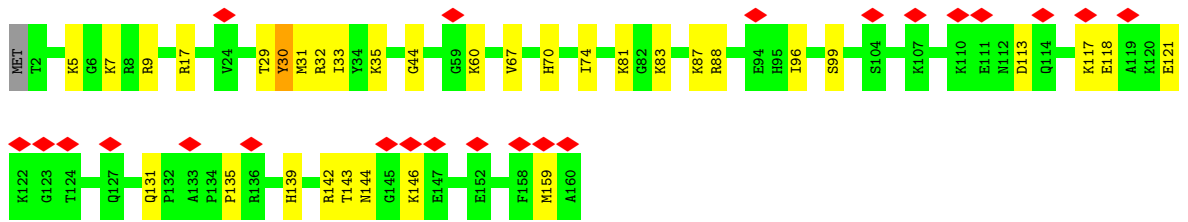
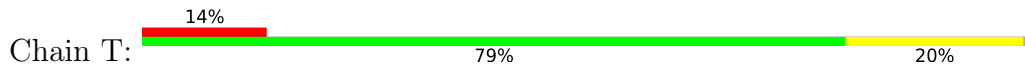
• Molecule 17: eL19



• Molecule 18: eL20

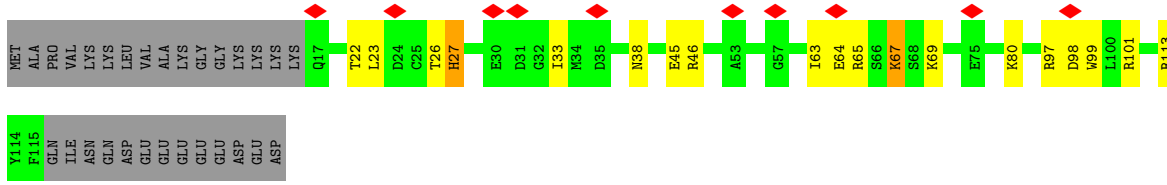


• Molecule 19: eL21

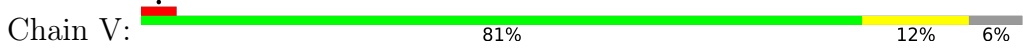


• Molecule 20: eL22

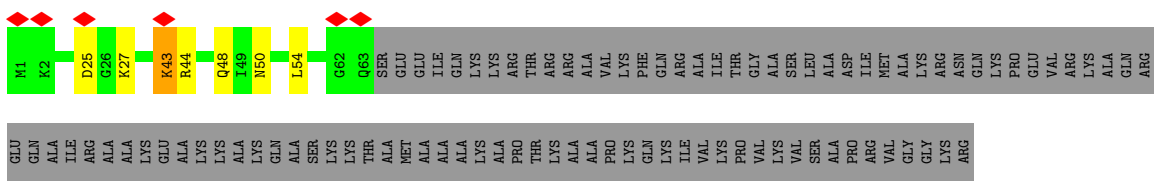




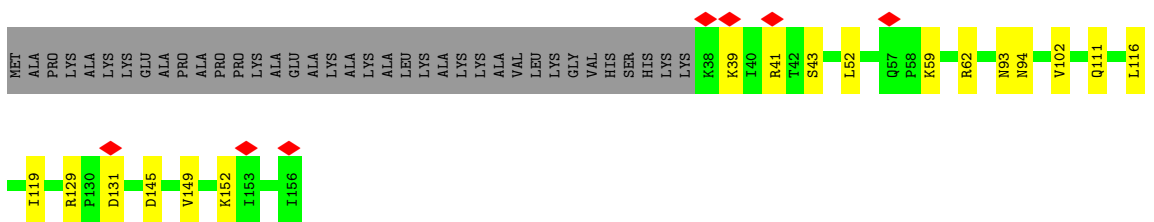
• Molecule 21: uL14



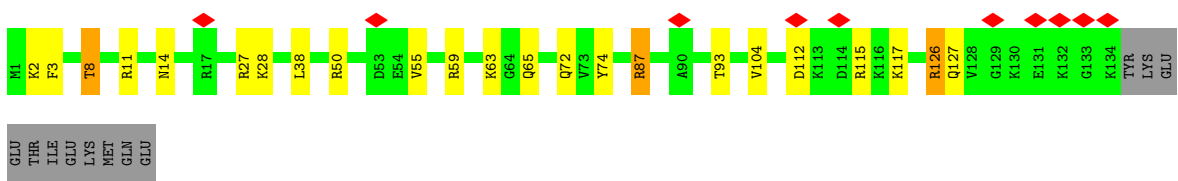
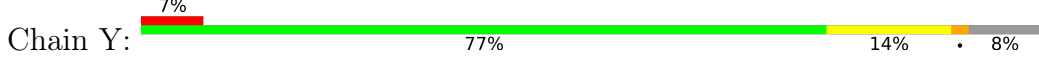
• Molecule 22: eL24



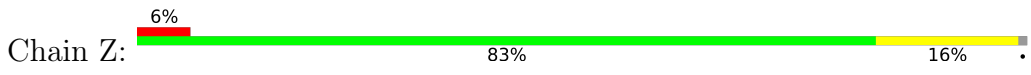
• Molecule 23: uL23

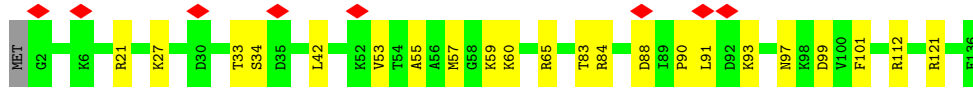


• Molecule 24: uL24

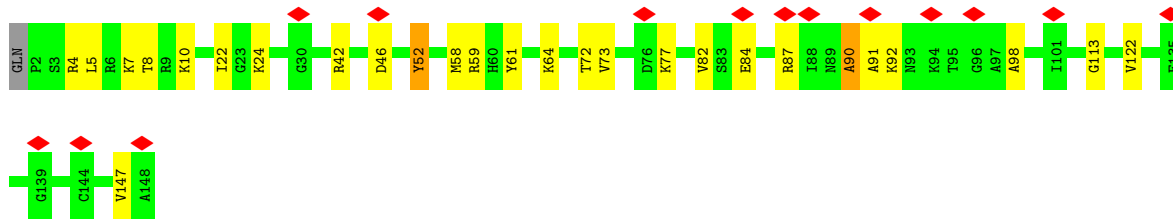
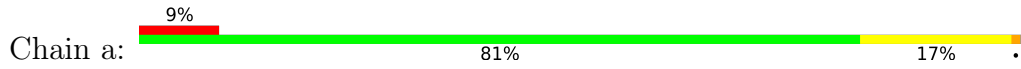


• Molecule 25: eL27

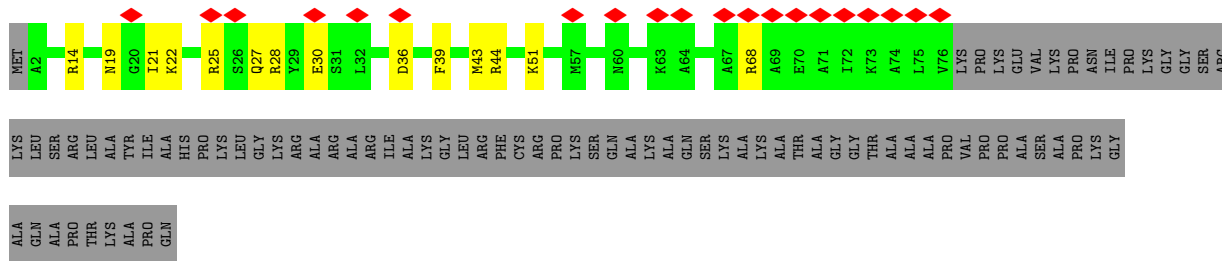
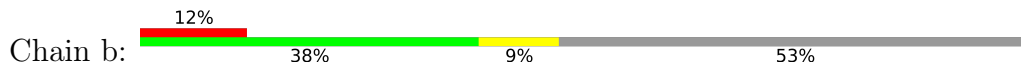




• Molecule 26: uL15



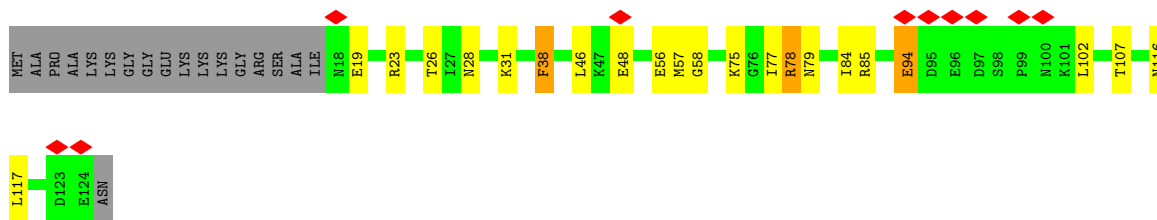
• Molecule 27: eL29



• Molecule 28: eL30



• Molecule 29: eL31

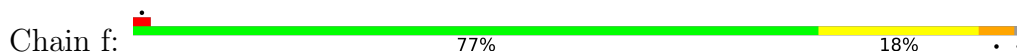


• Molecule 30: eL32

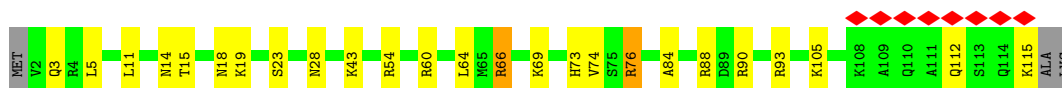
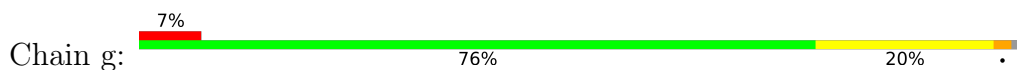




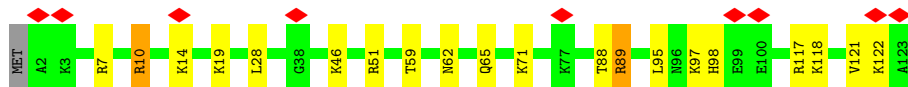
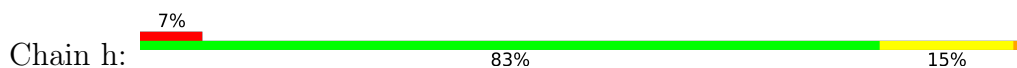
• Molecule 31: eL33



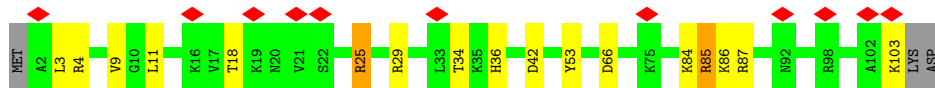
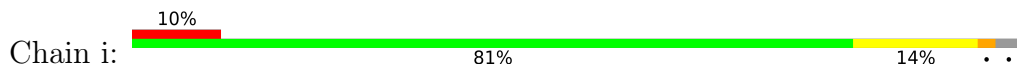
• Molecule 32: eL34



• Molecule 33: uL29



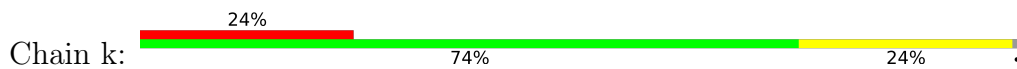
• Molecule 34: eL36

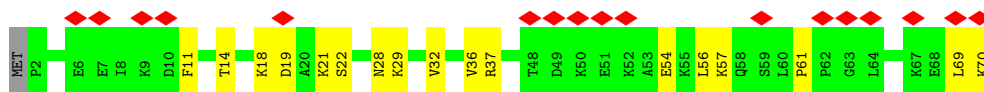


• Molecule 35: eL37

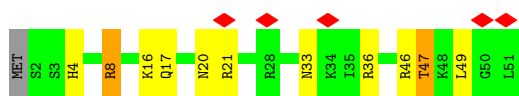
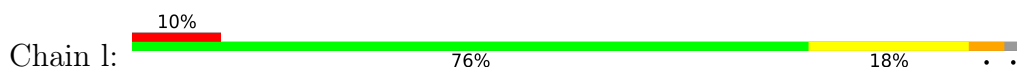


• Molecule 36: eL38

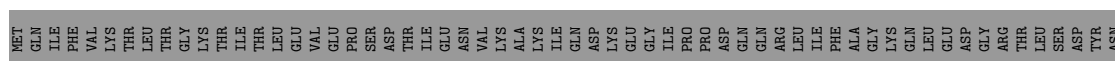




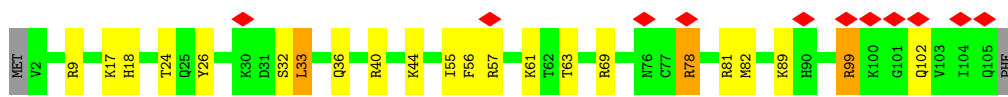
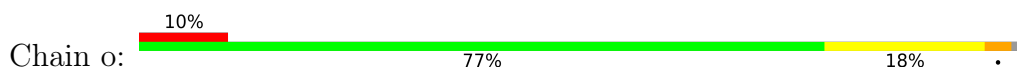
• Molecule 37: eL39



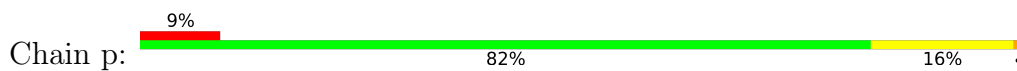
• Molecule 38: eL40



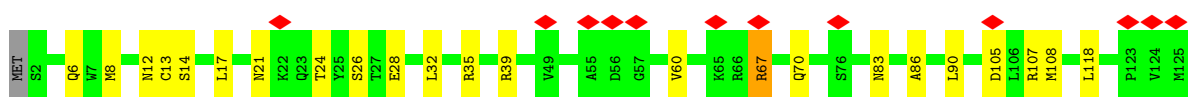
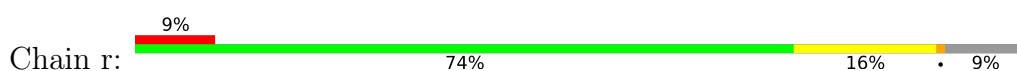
• Molecule 39: eL42



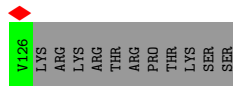
• Molecule 40: eL43

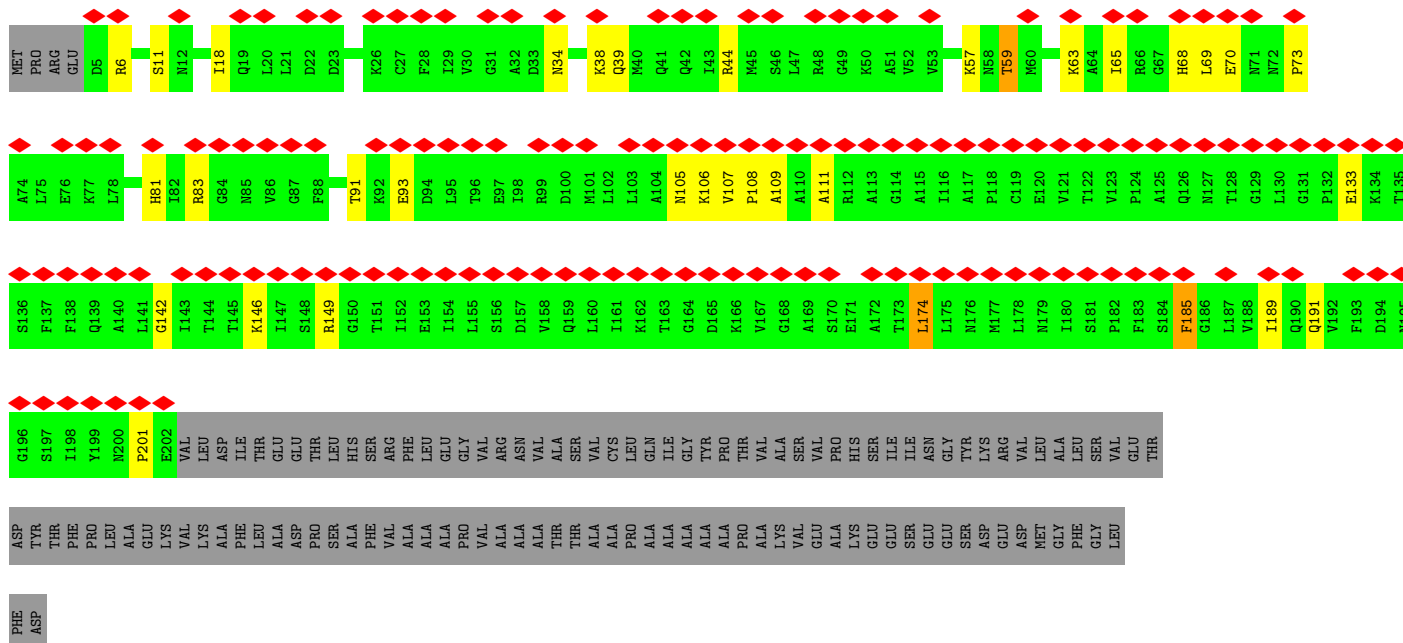


• Molecule 41: eL28

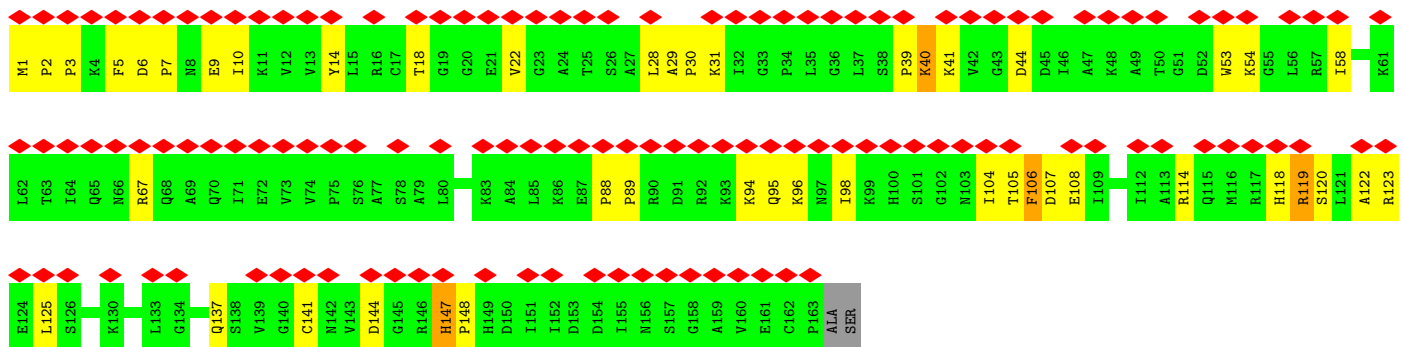
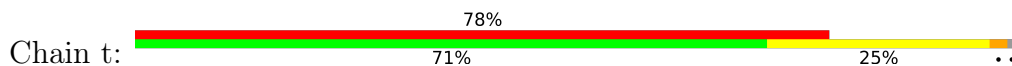


• Molecule 42: uL10

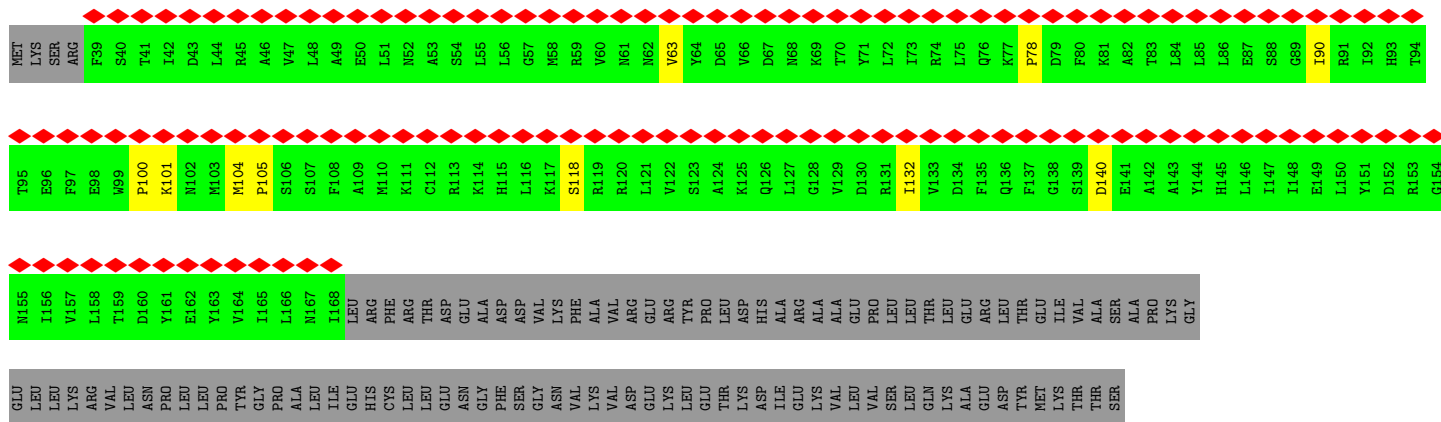




• Molecule 43: uL11



• Molecule 44: NEMF







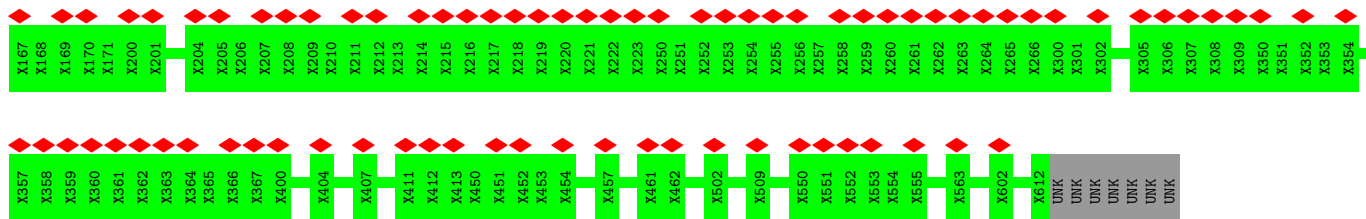




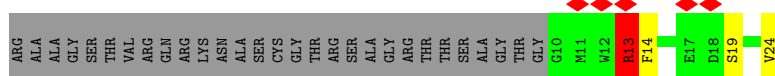




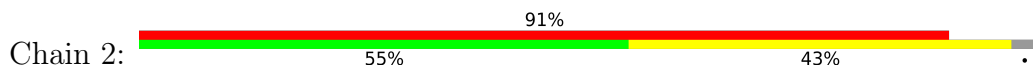




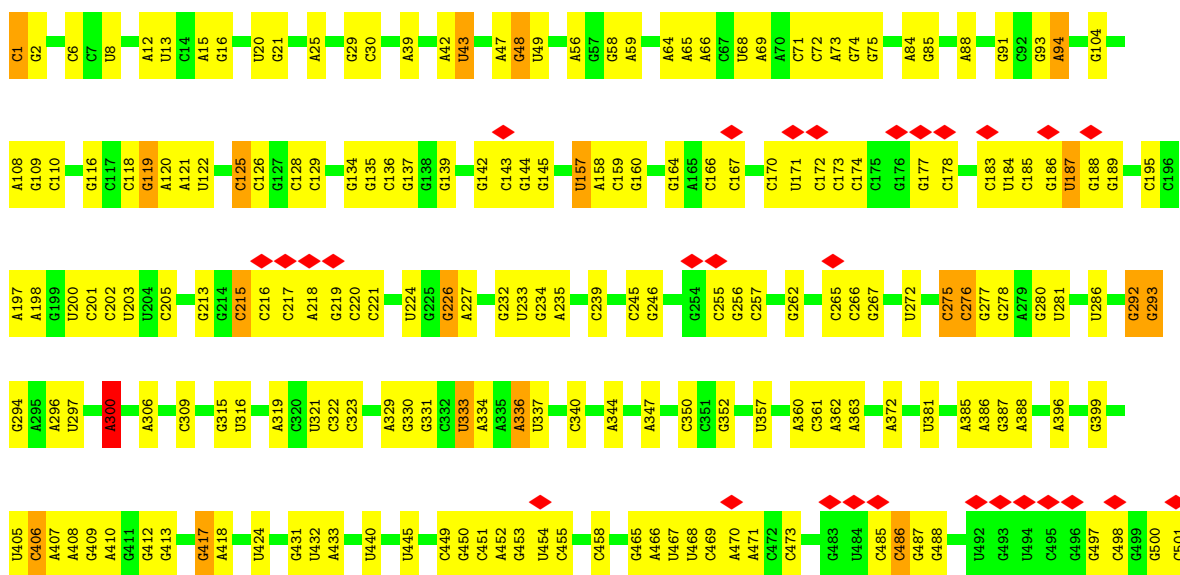
• Molecule 47: nascent chain

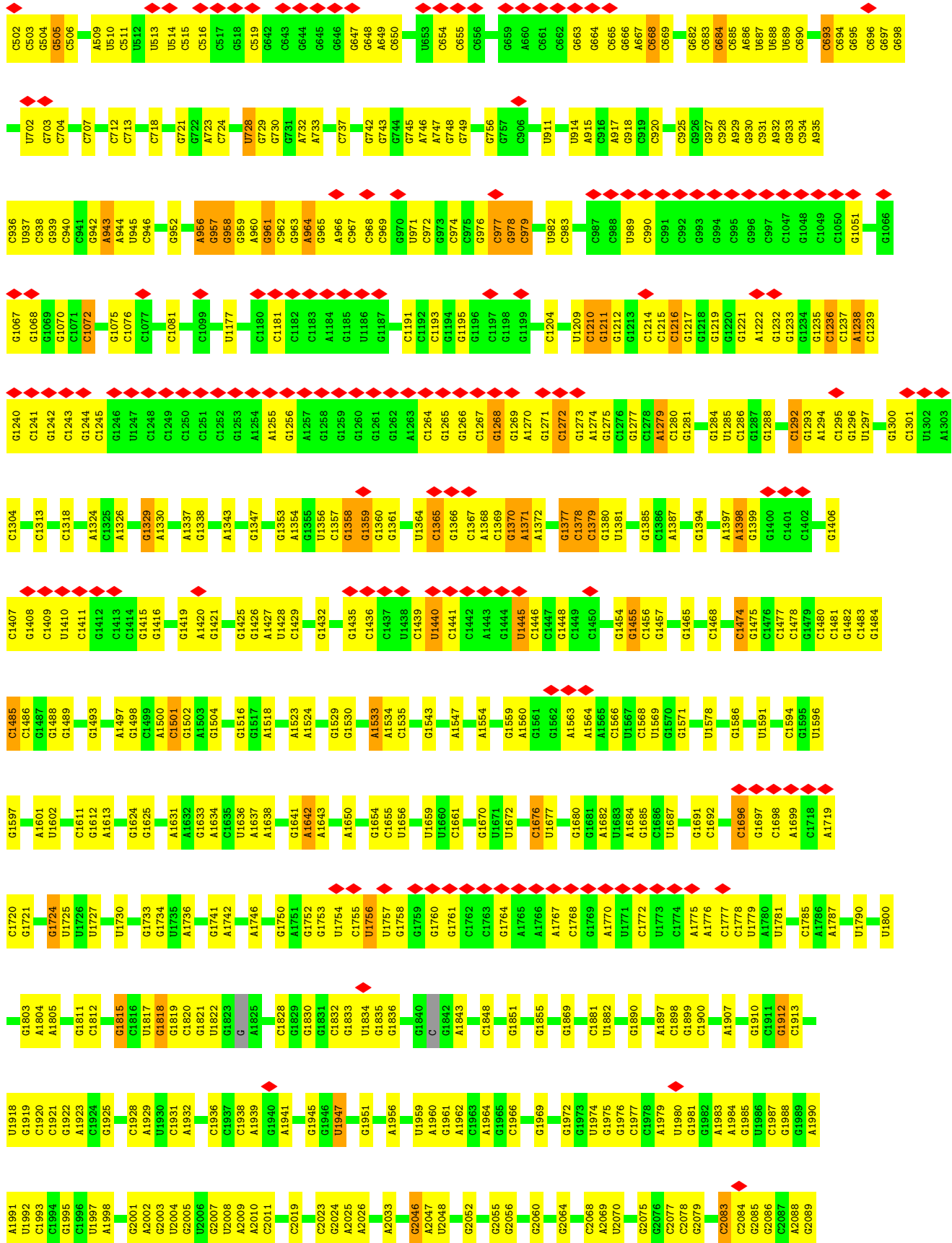


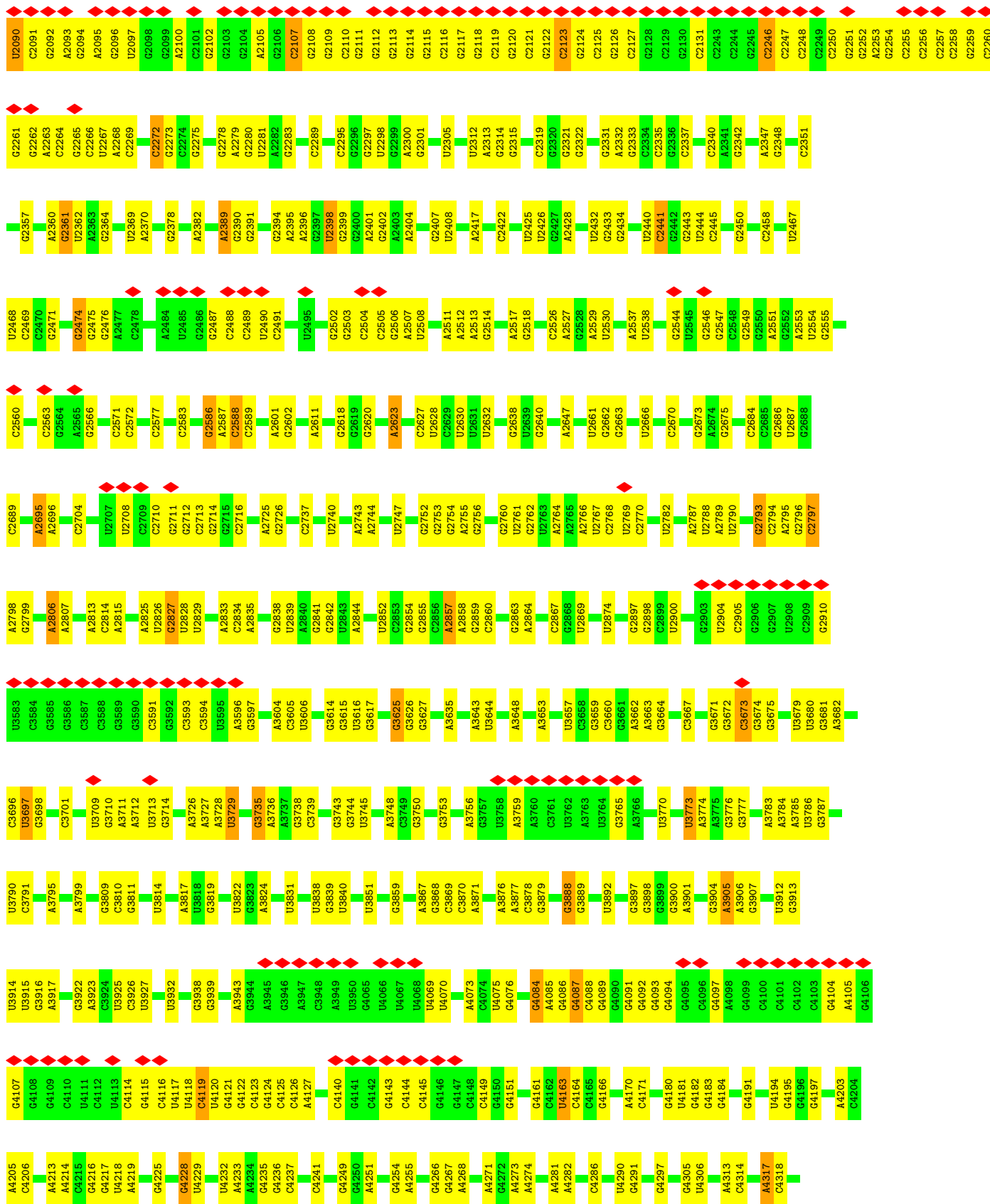
• Molecule 48: tRNA



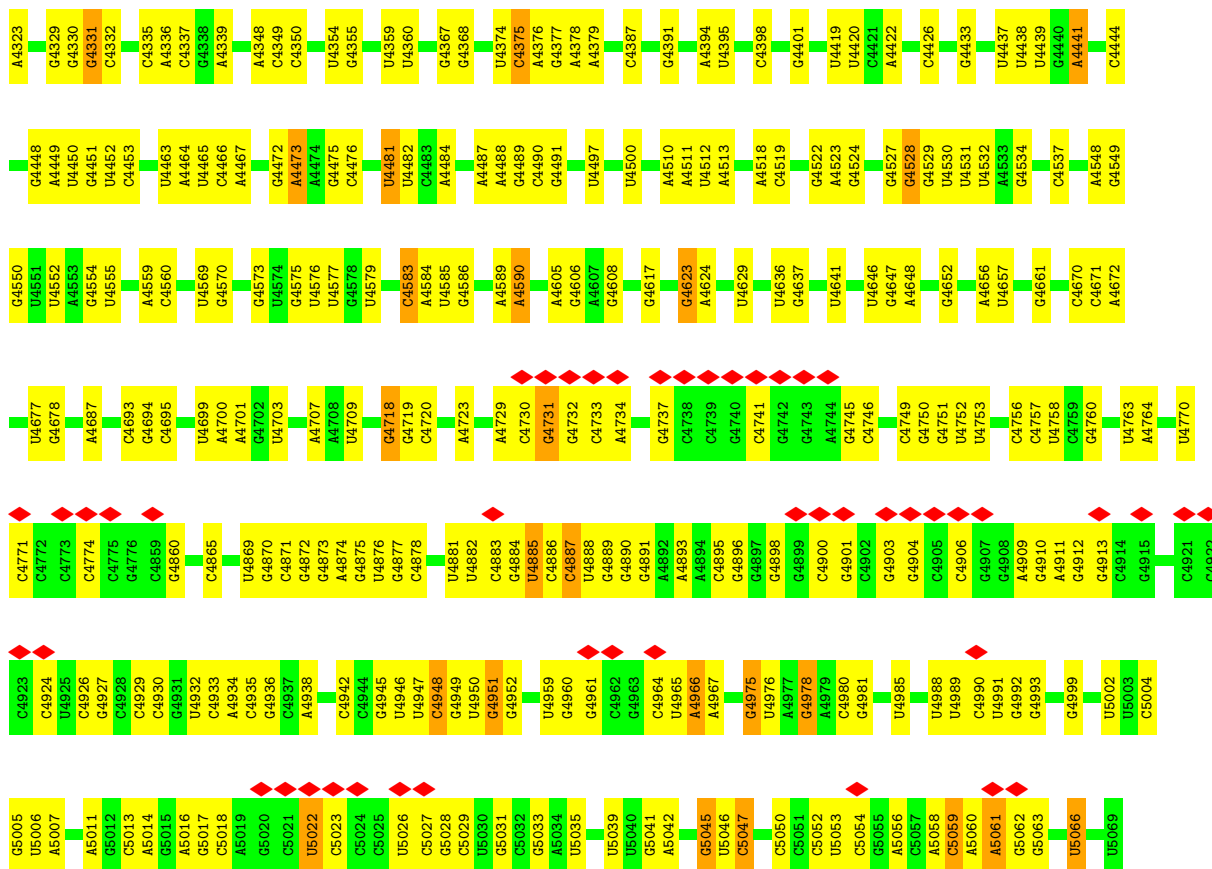
• Molecule 49: 28S rRNA



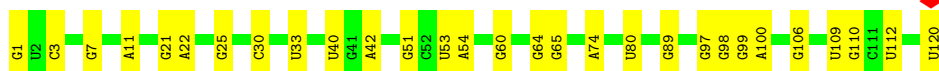
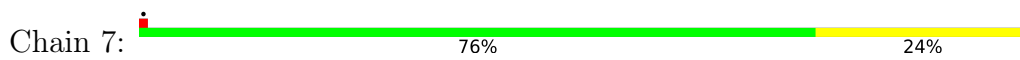




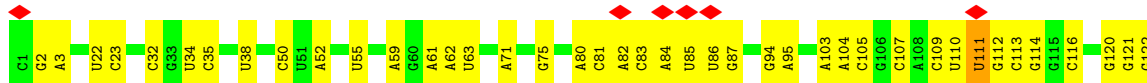




• Molecule 50: 5S rRNA



• Molecule 51: 5.8S rRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63826	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS, FEI TITAN KRIOS	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	2000, 2000	Depositor
Maximum defocus (nm)	3500, 3500	Depositor
Magnification	104478, 104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.494	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.08	Depositor
Map size ( $\text{\AA}$ )	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.34, 1.34, 1.34	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.59	0/1906	0.90	2/2556 (0.1%)
2	B	0.57	0/3214	0.88	1/4308 (0.0%)
3	C	0.61	0/2973	0.95	5/3990 (0.1%)
4	D	0.51	0/2430	0.85	3/3256 (0.1%)
5	E	0.52	0/1941	0.95	3/2601 (0.1%)
6	F	0.66	0/1905	1.00	4/2539 (0.2%)
7	G	0.51	0/1971	0.90	2/2652 (0.1%)
8	H	0.52	0/1537	0.91	1/2066 (0.0%)
9	I	0.56	0/1690	0.89	2/2257 (0.1%)
10	J	0.47	0/1382	0.83	1/1849 (0.1%)
11	L	0.59	0/1734	0.98	2/2318 (0.1%)
12	M	0.59	0/1152	0.89	0/1539
13	N	0.62	0/1746	0.97	0/2338
14	O	0.68	0/1671	1.01	1/2234 (0.0%)
15	P	0.62	0/1268	0.89	0/1701
16	Q	0.59	0/1530	0.99	1/2041 (0.0%)
17	R	0.51	0/1524	1.02	3/2013 (0.1%)
18	S	0.62	0/1493	0.97	3/2002 (0.1%)
19	T	0.60	0/1326	0.88	1/1770 (0.1%)
20	U	0.46	0/822	0.83	0/1103
21	V	0.59	0/993	0.86	0/1332
22	W	0.53	0/541	0.90	1/720 (0.1%)
23	X	0.50	0/993	0.85	0/1334
24	Y	0.53	0/1132	0.98	4/1504 (0.3%)
25	Z	0.51	0/1130	0.82	0/1507
26	a	0.68	0/1192	0.95	3/1591 (0.2%)
27	b	0.57	0/620	0.97	1/819 (0.1%)
28	c	0.51	0/742	0.78	0/996
29	d	0.58	0/903	1.03	3/1216 (0.2%)
30	e	0.62	0/1071	0.97	4/1429 (0.3%)
31	f	0.68	0/895	1.00	1/1198 (0.1%)
32	g	0.51	0/916	0.96	3/1220 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	h	0.51	0/1023	0.96	3/1350 (0.2%)
34	i	0.50	0/843	1.05	4/1115 (0.4%)
35	j	0.69	0/721	1.00	1/953 (0.1%)
36	k	0.41	0/575	0.83	0/761
37	l	0.57	0/454	0.98	1/599 (0.2%)
38	m	0.56	0/435	0.96	1/575 (0.2%)
39	o	0.53	0/864	0.90	1/1140 (0.1%)
40	p	0.54	0/718	0.89	1/953 (0.1%)
41	r	0.60	0/1017	0.96	0/1365
42	s	0.50	0/1546	0.77	2/2087 (0.1%)
43	t	0.52	0/1257	0.87	1/1697 (0.1%)
44	u	0.46	0/644	0.61	0/897
44	v	0.44	0/1099	0.82	1/1470 (0.1%)
45	0	0.53	0/301	0.69	0/400
45	w	0.47	0/110	0.78	0/146
45	z	0.45	0/1076	0.80	0/1451
47	1	0.59	0/129	0.83	0/173
48	2	0.26	0/1765	0.73	0/2749
49	5	0.49	11/87791 (0.0%)	0.88	177/136941 (0.1%)
50	7	0.42	0/2858	0.72	1/4455 (0.0%)
51	8	0.45	1/3701 (0.0%)	0.77	1/5766 (0.0%)
All	All	0.52	12/155270 (0.0%)	0.88	250/229042 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	4
3	C	0	2
4	D	0	1
5	E	0	4
6	F	0	1
7	G	0	2
8	H	0	1
9	I	0	3
11	L	0	2
13	N	0	1
14	O	0	1
17	R	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	S	0	3
19	T	0	3
21	V	0	1
24	Y	0	1
25	Z	0	1
26	a	0	2
27	b	0	1
31	f	0	2
33	h	0	1
34	i	0	1
36	k	0	1
42	s	0	2
43	t	0	4
47	l	0	1
49	5	0	3
All	All	0	52

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	5	957	G	O3'-P	8.72	1.71	1.61
49	5	1358	G	O3'-P	7.41	1.70	1.61
49	5	956	A	O3'-P	7.15	1.69	1.61
49	5	1370	G	O3'-P	6.23	1.68	1.61
49	5	4375	C	O3'-P	-5.70	1.54	1.61
49	5	293	G	O3'-P	-5.40	1.54	1.61
49	5	2394	G	O3'-P	-5.39	1.54	1.61
49	5	2086	G	O3'-P	-5.20	1.54	1.61
49	5	4087	G	O3'-P	-5.14	1.54	1.61
51	8	150	C	O3'-P	-5.14	1.54	1.61
49	5	372	A	O3'-P	-5.12	1.55	1.61
49	5	1659	U	O3'-P	-5.10	1.55	1.61

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	5	1358	G	C4'-C3'-O3'	11.60	136.20	113.00
24	Y	87	ARG	NE-CZ-NH2	10.23	125.41	120.30
34	i	25	ARG	NE-CZ-NH1	10.20	125.40	120.30
18	S	83	ARG	NE-CZ-NH2	9.56	125.08	120.30
49	5	336	A	O4'-C1'-N9	9.31	115.65	108.20
49	5	958	G	C2'-C3'-O3'	9.21	129.76	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	44	ARG	NE-CZ-NH1	9.14	124.87	120.30
49	5	336	A	C8-N9-C1'	-8.84	111.79	127.70
49	5	1455	G	C2'-C3'-O3'	8.83	128.93	109.50
49	5	336	A	C4-N9-C1'	8.81	142.16	126.30
49	5	977	C	C2'-C3'-O3'	8.80	128.86	109.50
49	5	215	C	C2'-C3'-O3'	8.69	128.62	109.50
49	5	336	A	C1'-O4'-C4'	-8.45	103.14	109.90
49	5	125	C	C2'-C3'-O3'	8.40	127.98	109.50
49	5	2389	A	C2'-C3'-O3'	8.39	127.95	109.50
49	5	4528	G	C2'-C3'-O3'	8.35	127.87	109.50
49	5	4948	C	C2'-C3'-O3'	8.35	127.87	109.50
49	5	1474	C	C2'-C3'-O3'	8.28	127.72	109.50
49	5	1356	U	C2'-C3'-O3'	8.22	127.60	109.50
49	5	2695	A	C2'-C3'-O3'	8.15	127.43	109.50
49	5	1501	C	N1-C1'-C2'	8.13	124.57	114.00
49	5	1211	G	C2'-C3'-O3'	8.10	127.33	109.50
49	5	293	G	C2'-C3'-O3'	8.09	127.30	109.50
6	F	238	ARG	N-CA-C	-8.05	89.25	111.00
49	5	1279	A	C2'-C3'-O3'	7.91	126.89	109.50
49	5	4887	C	C2'-C3'-O3'	7.89	126.87	109.50
3	C	342	ARG	NE-CZ-NH1	7.78	124.19	120.30
29	d	38	PHE	CB-CG-CD1	7.78	126.24	120.80
32	g	66	ARG	NE-CZ-NH1	7.75	124.18	120.30
49	5	406	C	C2'-C3'-O3'	7.75	126.55	109.50
26	a	61	TYR	N-CA-C	7.74	131.89	111.00
49	5	978	G	C2'-C3'-O3'	7.73	126.51	109.50
49	5	979	C	C2'-C3'-O3'	7.67	126.37	109.50
49	5	1292	C	C2'-C3'-O3'	7.66	126.35	109.50
49	5	4885	U	C2'-C3'-O3'	7.64	126.30	109.50
6	F	91	LEU	CA-CB-CG	7.63	132.84	115.30
49	5	2272	C	C2'-C3'-O3'	7.61	126.25	109.50
49	5	1696	C	C2'-C3'-O3'	7.57	126.16	109.50
49	5	2797	C	N1-C1'-C2'	-7.57	103.67	112.00
29	d	38	PHE	CB-CG-CD2	-7.57	115.50	120.80
49	5	1329	G	C2'-C3'-O3'	7.56	126.13	109.50
49	5	1379	C	N1-C1'-C2'	7.56	123.82	114.00
33	h	89	ARG	NE-CZ-NH1	7.50	124.05	120.30
49	5	48	G	C2'-C3'-O3'	7.46	125.91	109.50
30	e	46	ARG	NE-CZ-NH1	7.45	124.03	120.30
34	i	85	ARG	NE-CZ-NH1	7.42	124.01	120.30
8	H	125	ARG	NE-CZ-NH1	7.39	124.00	120.30
49	5	728	U	C2'-C3'-O3'	7.39	125.75	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	5	3625	G	C2'-C3'-O3'	7.37	125.70	109.50
49	5	1359	G	C2'-C3'-O3'	7.26	125.46	109.50
49	5	2246	C	C2'-C3'-O3'	7.25	125.44	109.50
49	5	668	C	C2'-C3'-O3'	7.20	125.34	109.50
49	5	4228	G	C2'-C3'-O3'	7.18	125.29	109.50
49	5	2632	U	N1-C1'-C2'	7.16	123.31	114.00
49	5	2083	C	C4'-C3'-O3'	7.13	127.27	113.00
49	5	4951	G	C2'-C3'-O3'	7.12	125.16	109.50
39	o	78	ARG	NE-CZ-NH2	7.08	123.84	120.30
7	G	163	PRO	N-CA-C	-7.06	93.75	112.10
49	5	5061	A	C2'-C3'-O3'	7.05	125.00	109.50
29	d	78	ARG	NE-CZ-NH1	7.04	123.82	120.30
49	5	3888	G	C2'-C3'-O3'	7.00	124.89	113.70
49	5	1370	G	N9-C1'-C2'	6.99	123.09	114.00
49	5	4163	U	C4'-C3'-O3'	6.96	126.92	113.00
50	7	1	G	C5'-C4'-O4'	6.94	117.42	109.10
40	p	85	ARG	NE-CZ-NH1	6.92	123.76	120.30
49	5	293	G	C4'-C3'-O3'	-6.91	94.89	109.40
49	5	1379	C	O4'-C1'-N1	6.91	113.73	108.20
49	5	276	C	C2'-C3'-O3'	6.88	124.70	113.70
49	5	958	G	O5'-P-OP2	-6.81	99.57	105.70
2	B	261	ARG	N-CA-C	-6.77	92.73	111.00
49	5	2046	G	C2'-C3'-O3'	6.74	124.49	113.70
49	5	226	G	C2'-C3'-O3'	6.74	124.48	113.70
5	E	101	ARG	NE-CZ-NH2	6.73	123.66	120.30
49	5	505	G	C2'-C3'-O3'	6.69	124.40	113.70
26	a	113	GLY	N-CA-C	6.66	129.74	113.10
49	5	5059	C	C2'-C3'-O3'	6.64	124.33	113.70
49	5	1676	C	O5'-P-OP2	-6.63	99.73	105.70
49	5	300	A	N9-C1'-C2'	6.62	122.60	114.00
49	5	3697	U	C2'-C3'-O3'	6.60	124.26	113.70
49	5	1379	C	C1'-O4'-C4'	-6.59	104.63	109.90
49	5	2827	G	C2'-C3'-O3'	-6.58	95.03	109.50
49	5	1947	U	C4'-C3'-O3'	6.57	126.14	113.00
49	5	4473	A	N9-C1'-C2'	6.55	122.52	114.00
49	5	2857	A	N9-C1'-C2'	-6.51	104.84	112.00
49	5	1	C	C5'-C4'-O4'	6.51	116.91	109.10
49	5	4331	G	C2'-C3'-O3'	6.49	124.09	113.70
49	5	275	C	C2'-C3'-O3'	6.49	124.08	113.70
49	5	1398	A	C2'-C3'-O3'	6.47	124.06	113.70
49	5	94	A	N9-C1'-C2'	6.44	122.37	114.00
49	5	2588	C	C4'-C3'-O3'	6.39	125.79	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	5	43	U	O4'-C4'-C3'	-6.35	97.65	104.00
49	5	4481	U	C5'-C4'-O4'	6.33	116.69	109.10
49	5	1365	C	C4'-C3'-O3'	6.30	125.60	113.00
49	5	1371	A	O4'-C1'-C2'	-6.29	99.52	105.80
49	5	286	U	N1-C1'-C2'	6.28	122.17	114.00
49	5	3773	U	C2'-C3'-O3'	6.20	123.61	113.70
49	5	4723	A	C4-N9-C1'	6.14	137.35	126.30
49	5	4723	A	C8-N9-C1'	-6.14	116.65	127.70
18	S	87	ARG	NE-CZ-NH1	6.13	123.36	120.30
49	5	4731	G	N9-C1'-C2'	6.13	121.97	114.00
51	8	111	U	C2'-C3'-O3'	6.12	123.50	113.70
49	5	1485	C	C2'-C3'-O3'	6.10	123.46	113.70
30	e	46	ARG	NE-CZ-NH2	-6.06	117.27	120.30
49	5	1501	C	O4'-C1'-N1	6.06	113.05	108.20
49	5	4978	G	C5'-C4'-O4'	6.05	116.36	109.10
49	5	5066	U	N1-C1'-C2'	6.04	121.84	114.00
24	Y	126	ARG	NE-CZ-NH1	6.03	123.32	120.30
31	f	36	ARG	NE-CZ-NH1	6.01	123.31	120.30
49	5	1682	A	C8-N9-C1'	-6.01	116.88	127.70
49	5	1682	A	C4-N9-C1'	6.00	137.11	126.30
49	5	961	G	C2'-C3'-O3'	-5.99	96.32	109.50
34	i	25	ARG	NE-CZ-NH2	-5.99	117.31	120.30
49	5	333	U	C4'-C3'-O3'	5.94	124.88	113.00
24	Y	8	THR	N-CA-C	5.94	127.03	111.00
33	h	89	ARG	CG-CD-NE	5.92	124.23	111.80
49	5	1642	A	C2'-C3'-O3'	5.91	123.16	113.70
1	A	196	TRP	C-N-CD	5.90	140.79	128.40
49	5	1818	G	C2'-C3'-O3'	5.90	123.14	113.70
49	5	1072	C	N1-C1'-C2'	5.87	121.64	114.00
49	5	300	A	C8-N9-C1'	-5.86	117.15	127.70
49	5	30	C	O5'-P-OP2	-5.81	100.47	105.70
49	5	1440	U	C2'-C3'-O3'	5.78	122.95	113.70
49	5	1210	C	N1-C1'-C2'	5.75	121.47	114.00
18	S	95	ARG	NE-CZ-NH1	5.74	123.17	120.30
49	5	292	G	C4'-C3'-O3'	5.73	124.46	113.00
9	I	92	HIS	N-CA-C	-5.71	95.57	111.00
49	5	957	G	P-O3'-C3'	5.70	126.54	119.70
17	R	103	ARG	NE-CZ-NH1	5.68	123.14	120.30
49	5	3773	U	C4'-C3'-O3'	5.67	124.35	113.00
49	5	943	A	N9-C1'-C2'	-5.67	105.77	112.00
49	5	1724	G	N9-C1'-C2'	5.67	121.37	114.00
49	5	300	A	C4-N9-C1'	5.67	136.50	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	v	406	VAL	N-CA-C	-5.65	95.74	111.00
49	5	1236	C	C2'-C3'-O3'	5.64	122.72	113.70
49	5	1377	G	C2'-C3'-O3'	5.64	122.72	113.70
6	F	43	MET	CB-CG-SD	5.62	129.26	112.40
1	A	9	ARG	NE-CZ-NH1	5.61	123.10	120.30
49	5	2586	G	N9-C1'-C2'	5.60	121.28	114.00
49	5	486	C	C2'-C3'-O3'	5.59	122.65	113.70
49	5	1268	G	N9-C1'-C2'	5.59	121.27	114.00
49	5	1238	A	C2'-C3'-O3'	5.59	122.64	113.70
49	5	956	A	C2'-C3'-O3'	5.57	122.62	113.70
49	5	3673	C	C2'-C3'-O3'	5.57	122.62	113.70
43	t	88	PRO	C-N-CD	-5.56	108.37	120.60
49	5	4228	G	C4'-C3'-O3'	-5.55	97.75	109.40
49	5	4084	G	C2'-C3'-O3'	5.54	122.56	113.70
49	5	2623	A	C8-N9-C1'	-5.53	117.75	127.70
49	5	1359	G	N9-C1'-C2'	5.52	121.18	114.00
42	s	174	LEU	CA-CB-CG	5.52	127.99	115.30
49	5	2623	A	C4-N9-C1'	5.52	136.24	126.30
49	5	4975	G	C1'-O4'-C4'	-5.51	105.49	109.90
49	5	1533	A	C2'-C3'-O3'	5.50	122.50	113.70
17	R	107	ARG	NE-CZ-NH1	5.50	123.05	120.30
26	a	64	LYS	N-CA-C	-5.49	96.17	111.00
49	5	3735	G	C2'-C3'-O3'	5.49	122.48	113.70
49	5	3729	U	N1-C1'-C2'	5.48	121.13	114.00
49	5	964	A	C4'-C3'-O3'	5.47	123.94	113.00
27	b	14	ARG	NE-CZ-NH2	5.47	123.03	120.30
49	5	1672	U	C2-N1-C1'	5.43	124.22	117.70
49	5	2586	G	O4'-C1'-N9	5.43	112.54	108.20
49	5	5022	U	C2'-C3'-O3'	5.43	122.39	113.70
49	5	1815	G	N9-C1'-C2'	5.42	121.05	114.00
49	5	2806	A	O4'-C1'-N9	5.41	112.53	108.20
49	5	4590	A	O5'-P-OP1	-5.40	100.84	105.70
49	5	964	A	O4'-C1'-C2'	-5.39	100.41	105.80
49	5	2398	U	C2'-C3'-O3'	5.39	122.33	113.70
17	R	103	ARG	NE-CZ-NH2	-5.39	117.61	120.30
49	5	4181	U	C2'-C3'-O3'	5.37	122.29	113.70
49	5	956	A	P-O3'-C3'	5.37	126.14	119.70
49	5	187	U	C2'-C3'-O3'	5.36	122.27	113.70
49	5	1501	C	C1'-O4'-C4'	-5.36	105.61	109.90
49	5	3773	U	N1-C1'-C2'	-5.36	106.11	112.00
6	F	72	ARG	NE-CZ-NH1	5.36	122.98	120.30
37	l	8	ARG	NE-CZ-NH1	5.35	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	5	693	C	C2'-C3'-O3'	5.34	122.25	113.70
49	5	5047	C	C2'-C3'-O3'	5.34	122.24	113.70
49	5	2060	G	C2'-C3'-O3'	5.32	122.22	113.70
9	I	139	ARG	NE-CZ-NH1	5.32	122.96	120.30
5	E	212	TYR	CA-CB-CG	5.31	123.49	113.40
49	5	1427	A	C2'-C3'-O3'	5.30	122.18	113.70
49	5	1730	U	C2'-C3'-O3'	5.30	122.18	113.70
3	C	98	GLY	N-CA-C	-5.30	99.86	113.10
49	5	4281	A	C1'-O4'-C4'	-5.30	105.66	109.90
49	5	47	A	C2'-C3'-O3'	-5.29	97.87	109.50
49	5	977	C	O4'-C4'-C3'	-5.28	98.72	104.00
49	5	1272	C	O4'-C1'-N1	5.28	112.42	108.20
49	5	4623	G	O5'-P-OP2	-5.28	100.95	105.70
49	5	4623	G	O5'-P-OP1	5.27	117.02	110.70
49	5	1361	G	C2'-C3'-O3'	5.26	122.12	113.70
49	5	2441	C	O5'-P-OP1	-5.26	100.96	105.70
10	J	145	LYS	N-CA-C	5.26	125.21	111.00
11	L	36	ARG	NE-CZ-NH1	5.26	122.93	120.30
49	5	1912	G	C2'-C3'-O3'	5.26	122.11	113.70
49	5	2090	U	C5'-C4'-O4'	5.26	115.41	109.10
42	s	59	THR	N-CA-C	-5.25	96.83	111.00
49	5	1216	C	C2'-C3'-O3'	5.23	122.06	113.70
49	5	2107	C	C2'-C3'-O3'	5.22	122.06	113.70
3	C	204	ARG	NE-CZ-NH2	5.22	122.91	120.30
49	5	2332	A	C4'-C3'-O3'	-5.20	98.48	109.40
7	G	127	ASP	CB-CG-OD2	5.19	122.97	118.30
35	j	11	ARG	NE-CZ-NH1	5.19	122.89	120.30
49	5	977	C	C5'-C4'-O4'	5.18	115.32	109.10
49	5	1752	G	C1'-O4'-C4'	-5.18	105.75	109.90
49	5	2474	G	C2'-C3'-O3'	5.18	121.99	113.70
24	Y	87	ARG	NE-CZ-NH1	-5.18	117.71	120.30
49	5	684	G	C2'-C3'-O3'	5.17	121.97	113.70
49	5	43	U	C5'-C4'-O4'	5.16	115.29	109.10
49	5	4718	G	N9-C1'-C2'	-5.16	106.33	112.00
49	5	43	U	O4'-C1'-N1	5.16	112.33	108.20
14	O	120	VAL	C-N-CD	5.15	139.22	128.40
16	Q	158	THR	N-CA-C	-5.15	97.10	111.00
38	m	97	ARG	NE-CZ-NH2	5.15	122.87	120.30
49	5	466	A	C4-N9-C1'	5.14	135.56	126.30
4	D	35	ARG	NE-CZ-NH1	5.14	122.87	120.30
19	T	30	TYR	CA-CB-CG	5.13	123.15	113.40
49	5	1378	C	N1-C1'-C2'	5.12	120.66	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	5	4966	A	N9-C1'-C2'	5.11	120.65	114.00
3	C	342	ARG	CG-CD-NE	5.11	122.52	111.80
33	h	89	ARG	NE-CZ-NH2	-5.11	117.75	120.30
49	5	4119	C	C2'-C3'-O3'	5.09	121.85	113.70
11	L	78	LEU	CA-CB-CG	-5.09	103.59	115.30
49	5	417	G	O4'-C1'-N9	5.08	112.26	108.20
32	g	66	ARG	NE-CZ-NH2	-5.08	117.76	120.30
34	i	85	ARG	CG-CD-NE	5.07	122.44	111.80
49	5	4579	U	N1-C1'-C2'	5.07	120.59	114.00
30	e	55	MET	C-N-CD	5.07	139.04	128.40
49	5	3905	A	C2'-C3'-O3'	5.06	121.79	113.70
32	g	76	ARG	NE-CZ-NH1	5.05	122.83	120.30
49	5	5045	G	C2'-C3'-O3'	5.05	121.78	113.70
49	5	30	C	O5'-P-OP1	5.05	116.76	110.70
49	5	1343	A	C2'-C3'-O3'	5.05	121.78	113.70
49	5	4583	C	N1-C1'-C2'	-5.04	106.45	112.00
49	5	119	G	O4'-C4'-C3'	-5.04	98.96	104.00
49	5	1445	U	C2'-C3'-O3'	5.04	121.76	113.70
49	5	2361	G	C2'-C3'-O3'	5.04	121.76	113.70
49	5	157	U	C1'-O4'-C4'	-5.04	105.87	109.90
49	5	4473	A	C8-N9-C1'	-5.04	118.64	127.70
3	C	100	ARG	NE-CZ-NH2	-5.03	117.78	120.30
4	D	35	ARG	NE-CZ-NH2	-5.03	117.78	120.30
49	5	4317	A	C2'-C3'-O3'	5.03	121.75	113.70
49	5	2123	C	C2'-C3'-O3'	5.03	121.75	113.70
49	5	4441	A	P-O5'-C5'	-5.03	112.86	120.90
49	5	1756	U	N1-C1'-C2'	5.02	120.53	114.00
49	5	4331	G	C4'-C3'-O3'	-5.02	98.85	109.40
49	5	1501	C	O4'-C1'-C2'	-5.02	100.78	105.80
4	D	15	ARG	NE-CZ-NH2	5.01	122.81	120.30
49	5	4473	A	C4-N9-C1'	5.01	135.32	126.30
5	E	210	ASP	CB-CG-OD2	-5.01	113.79	118.30
30	e	46	ARG	CG-CD-NE	5.01	122.31	111.80
49	5	1672	U	C6-N1-C1'	-5.01	114.19	121.20

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	1	13	ARG	Peptide
49	5	1191	C	Sidechain
49	5	2793	G	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
49	5	300	A	Sidechain
1	A	131	GLY	Peptide
2	B	17	LEU	Peptide
2	B	257	TRP	Peptide
2	B	332	MET	Peptide
2	B	351	LEU	Peptide
3	C	131	SER	Peptide
3	C	339	THR	Peptide
4	D	160	PHE	Peptide
5	E	123	SER	Peptide
5	E	173	GLY	Peptide
5	E	196	LYS	Peptide
5	E	216	LYS	Peptide
6	F	148	ASN	Peptide
7	G	161	VAL	Peptide
7	G	238	GLY	Peptide
8	H	188	GLN	Peptide
9	I	143	GLN	Peptide
9	I	188	LYS	Peptide
9	I	204	GLY	Peptide
11	L	146	LEU	Peptide
11	L	66	TYR	Peptide
13	N	184	ILE	Peptide
14	O	200	GLY	Peptide
17	R	39	GLN	Peptide
17	R	93	VAL	Peptide
18	S	154	LEU	Peptide
18	S	164	LYS	Peptide
18	S	5	GLY	Peptide
19	T	135	PRO	Peptide
19	T	32	ARG	Peptide
19	T	87	LYS	Peptide
21	V	97	TYR	Peptide
24	Y	14	ASN	Peptide
25	Z	53	VAL	Peptide
26	a	46	ASP	Peptide
26	a	90	ALA	Peptide
27	b	19	ASN	Peptide
31	f	100	ARG	Peptide
31	f	106	TYR	Peptide
33	h	95	LEU	Peptide
34	i	42	ASP	Peptide

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Mol	Chain	Res	Type	Group
36	k	28	ASN	Peptide
42	s	6	ARG	Peptide
42	s	81	HIS	Peptide
43	t	147	HIS	Peptide
43	t	29	ALA	Peptide
43	t	6	ASP	Peptide
43	t	98	ILE	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/257 (94%)	203 (84%)	28 (12%)	11 (4%)	2	23
2	B	392/395 (99%)	342 (87%)	44 (11%)	6 (2%)	10	47
3	C	365/368 (99%)	315 (86%)	43 (12%)	7 (2%)	8	42
4	D	290/297 (98%)	266 (92%)	18 (6%)	6 (2%)	7	40
5	E	232/284 (82%)	176 (76%)	39 (17%)	17 (7%)	1	13
6	F	223/250 (89%)	203 (91%)	16 (7%)	4 (2%)	8	43
7	G	239/266 (90%)	196 (82%)	36 (15%)	7 (3%)	4	33
8	H	188/192 (98%)	164 (87%)	17 (9%)	7 (4%)	3	28
9	I	200/214 (94%)	171 (86%)	22 (11%)	7 (4%)	3	30
10	J	168/178 (94%)	143 (85%)	17 (10%)	8 (5%)	2	22
11	L	208/211 (99%)	174 (84%)	22 (11%)	12 (6%)	1	18
12	M	136/213 (64%)	118 (87%)	16 (12%)	2 (2%)	10	47
13	N	201/204 (98%)	172 (86%)	28 (14%)	1 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	O	197/204 (97%)	173 (88%)	23 (12%)	1 (0%)	29	68
15	P	151/184 (82%)	133 (88%)	17 (11%)	1 (1%)	22	61
16	Q	185/188 (98%)	161 (87%)	22 (12%)	2 (1%)	14	53
17	R	178/196 (91%)	160 (90%)	14 (8%)	4 (2%)	6	39
18	S	173/224 (77%)	153 (88%)	16 (9%)	4 (2%)	6	38
19	T	157/160 (98%)	136 (87%)	19 (12%)	2 (1%)	12	50
20	U	97/128 (76%)	84 (87%)	9 (9%)	4 (4%)	3	26
21	V	129/140 (92%)	112 (87%)	16 (12%)	1 (1%)	19	59
22	W	61/157 (39%)	55 (90%)	5 (8%)	1 (2%)	9	46
23	X	117/156 (75%)	105 (90%)	11 (9%)	1 (1%)	17	57
24	Y	132/145 (91%)	121 (92%)	9 (7%)	2 (2%)	10	47
25	Z	133/136 (98%)	115 (86%)	13 (10%)	5 (4%)	3	27
26	a	145/148 (98%)	118 (81%)	20 (14%)	7 (5%)	2	22
27	b	73/160 (46%)	68 (93%)	4 (6%)	1 (1%)	11	48
28	c	92/115 (80%)	86 (94%)	5 (5%)	1 (1%)	14	53
29	d	105/125 (84%)	93 (89%)	9 (9%)	3 (3%)	4	33
30	e	126/135 (93%)	113 (90%)	11 (9%)	2 (2%)	9	46
31	f	107/110 (97%)	93 (87%)	10 (9%)	4 (4%)	3	28
32	g	112/117 (96%)	98 (88%)	12 (11%)	2 (2%)	8	43
33	h	120/123 (98%)	103 (86%)	16 (13%)	1 (1%)	19	59
34	i	100/105 (95%)	92 (92%)	5 (5%)	3 (3%)	4	33
35	j	84/97 (87%)	70 (83%)	12 (14%)	2 (2%)	6	37
36	k	67/70 (96%)	56 (84%)	8 (12%)	3 (4%)	2	23
37	l	48/51 (94%)	38 (79%)	8 (17%)	2 (4%)	3	25
38	m	50/128 (39%)	45 (90%)	3 (6%)	2 (4%)	3	26
39	o	102/106 (96%)	88 (86%)	11 (11%)	3 (3%)	4	33
40	p	89/92 (97%)	74 (83%)	13 (15%)	2 (2%)	6	39
41	r	123/137 (90%)	102 (83%)	18 (15%)	3 (2%)	6	37
42	s	196/317 (62%)	159 (81%)	22 (11%)	15 (8%)	1	12
43	t	161/165 (98%)	93 (58%)	39 (24%)	29 (18%)	0	2
44	u	128/501 (26%)	88 (69%)	30 (23%)	10 (8%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	v	130/501 (26%)	125 (96%)	3 (2%)	2 (2%)	10	47
45	0	34/1766 (2%)	29 (85%)	3 (9%)	2 (6%)	1	18
45	w	13/1766 (1%)	13 (100%)	0	0	100	100
45	z	120/1766 (7%)	106 (88%)	10 (8%)	4 (3%)	4	31
47	1	13/104 (12%)	9 (69%)	1 (8%)	3 (23%)	0	0
All	All	7132/14052 (51%)	6110 (86%)	793 (11%)	229 (3%)	7	31

All (229) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	PHE
1	A	195	CYS
2	B	18	PRO
3	C	273	LEU
5	E	91	PRO
5	E	92	VAL
5	E	123	SER
5	E	174	PRO
5	E	175	LEU
5	E	221	PRO
7	G	128	VAL
7	G	161	VAL
8	H	40	HIS
8	H	105	ILE
8	H	110	SER
9	I	12	CYS
9	I	99	ILE
9	I	204	GLY
10	J	155	HIS
11	L	64	VAL
11	L	67	HIS
11	L	134	PRO
18	S	88	SER
18	S	165	PRO
23	X	131	ASP
25	Z	33	THR
25	Z	34	SER
25	Z	84	ARG
26	a	52	TYR
26	a	92	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
28	c	19	GLN
29	d	94	GLU
30	e	92	ASN
31	f	80	ASN
31	f	107	PRO
32	g	69	LYS
32	g	84	ALA
35	j	36	LYS
36	k	61	PRO
39	o	32	SER
41	r	107	ARG
42	s	69	LEU
42	s	111	ALA
42	s	201	PRO
43	t	5	PHE
43	t	9	GLU
43	t	30	PRO
43	t	31	LYS
43	t	39	PRO
43	t	53	TRP
43	t	89	PRO
43	t	106	PHE
43	t	147	HIS
43	t	148	PRO
44	u	78	PRO
44	u	90	ILE
44	u	100	PRO
44	u	101	LYS
44	u	105	PRO
44	u	132	ILE
44	v	404	ASN
45	z	1638	THR
45	z	1643	ASP
45	0	1743	SER
45	0	1762	ARG
47	1	13	ARG
47	1	14	PHE
1	A	20	VAL
3	C	16	GLU
3	C	73	VAL
3	C	194	GLY
3	C	195	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	275	SER
4	D	125	VAL
4	D	129	GLU
4	D	187	SER
5	E	95	ASP
5	E	118	PRO
5	E	151	GLY
5	E	234	GLU
6	F	148	ASN
7	G	45	ILE
9	I	187	LYS
10	J	124	GLY
10	J	152	GLY
11	L	47	ALA
11	L	143	GLU
12	M	89	THR
16	Q	14	ARG
17	R	19	LYS
17	R	130	ASN
19	T	44	GLY
20	U	97	ARG
20	U	98	ASP
26	a	4	ARG
29	d	58	GLY
29	d	116	ASN
31	f	79	GLY
33	h	10	ARG
34	i	9	VAL
36	k	22	SER
41	r	67	ARG
41	r	86	ALA
42	s	63	LYS
42	s	105	ASN
42	s	108	PRO
42	s	109	ALA
43	t	2	PRO
43	t	10	ILE
43	t	40	LYS
43	t	58	ILE
43	t	118	HIS
43	t	122	ALA
43	t	144	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
44	u	63	VAL
44	u	118	SER
45	z	1653	PRO
1	A	14	SER
1	A	67	TYR
1	A	130	SER
1	A	226	ARG
2	B	257	TRP
2	B	329	ASP
4	D	260	GLU
4	D	293	ARG
5	E	85	LEU
5	E	96	LYS
5	E	232	GLU
8	H	104	VAL
9	I	47	PRO
9	I	177	ASN
10	J	11	PRO
10	J	141	ILE
11	L	5	ARG
11	L	52	SER
11	L	176	PHE
17	R	36	ASN
20	U	67	LYS
22	W	43	LYS
24	Y	93	THR
35	j	21	ARG
37	l	49	LEU
38	m	107	ALA
40	p	41	PHE
42	s	34	ASN
42	s	57	LYS
42	s	93	GLU
42	s	185	PHE
43	t	54	LYS
43	t	119	ARG
1	A	127	ALA
1	A	180	LEU
2	B	123	HIS
3	C	309	ILE
5	E	115	GLU
5	E	218	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	224	GLN
5	E	229	PHE
7	G	125	LYS
8	H	22	GLY
8	H	108	ASN
8	H	140	GLN
10	J	150	CYS
11	L	172	GLU
16	Q	41	SER
18	S	155	PRO
24	Y	63	LYS
25	Z	55	ALA
26	a	91	ALA
30	e	127	ALA
34	i	3	LEU
34	i	11	LEU
37	l	47	THR
39	o	99	ARG
40	p	8	VAL
42	s	73	PRO
42	s	142	GLY
43	t	7	PRO
43	t	18	THR
43	t	28	LEU
43	t	105	THR
43	t	125	LEU
44	u	104	MET
44	u	140	ASP
45	z	1642	GLU
47	1	19	SER
2	B	116	ARG
6	F	105	PRO
6	F	175	ALA
7	G	123	ALA
9	I	201	PRO
11	L	63	THR
15	P	6	LEU
17	R	25	ASP
25	Z	90	PRO
26	a	90	ALA
26	a	98	ALA
42	s	106	LYS

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Mol	Chain	Res	Type
43	t	137	GLN
44	v	400	LYS
2	B	259	PRO
11	L	169	ILE
12	M	25	VAL
19	T	74	ILE
36	k	32	VAL
39	o	33	LEU
42	s	70	GLU
43	t	67	ARG
43	t	94	LYS
43	t	120	SER
1	A	212	GLY
1	A	213	GLY
7	G	186	GLY
11	L	100	PRO
13	N	137	PRO
26	a	22	ILE
31	f	64	PRO
4	D	47	PRO
10	J	174	ILE
20	U	27	HIS
6	F	230	VAL
7	G	238	GLY
14	O	30	GLY
21	V	22	VAL
10	J	176	PRO
27	b	21	ILE
43	t	3	PRO
18	S	172	PRO
38	m	78	ILE

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/199 (94%)	155 (83%)	32 (17%)	2	13
2	B	335/336 (100%)	285 (85%)	50 (15%)	3	19
3	C	305/306 (100%)	243 (80%)	62 (20%)	1	8
4	D	247/250 (99%)	207 (84%)	40 (16%)	2	15
5	E	209/246 (85%)	172 (82%)	37 (18%)	2	11
6	F	194/217 (89%)	156 (80%)	38 (20%)	1	8
7	G	208/226 (92%)	170 (82%)	38 (18%)	1	10
8	H	169/171 (99%)	135 (80%)	34 (20%)	1	8
9	I	174/181 (96%)	137 (79%)	37 (21%)	1	7
10	J	143/149 (96%)	124 (87%)	19 (13%)	4	23
11	L	176/177 (99%)	137 (78%)	39 (22%)	1	6
12	M	116/160 (72%)	95 (82%)	21 (18%)	1	11
13	N	171/172 (99%)	142 (83%)	29 (17%)	2	14
14	O	171/174 (98%)	149 (87%)	22 (13%)	4	24
15	P	134/163 (82%)	110 (82%)	24 (18%)	2	11
16	Q	163/164 (99%)	137 (84%)	26 (16%)	2	16
17	R	159/175 (91%)	126 (79%)	33 (21%)	1	7
18	S	156/192 (81%)	125 (80%)	31 (20%)	1	8
19	T	139/140 (99%)	111 (80%)	28 (20%)	1	8
20	U	89/114 (78%)	72 (81%)	17 (19%)	1	9
21	V	101/107 (94%)	86 (85%)	15 (15%)	3	19
22	W	55/126 (44%)	49 (89%)	6 (11%)	6	32
23	X	107/133 (80%)	91 (85%)	16 (15%)	3	19
24	Y	124/135 (92%)	104 (84%)	20 (16%)	2	16
25	Z	117/118 (99%)	101 (86%)	16 (14%)	3	22
26	a	119/120 (99%)	102 (86%)	17 (14%)	3	21
27	b	63/123 (51%)	52 (82%)	11 (18%)	2	12
28	c	79/97 (81%)	69 (87%)	10 (13%)	4	24
29	d	98/110 (89%)	78 (80%)	20 (20%)	1	8
30	e	114/121 (94%)	83 (73%)	31 (27%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	f	88/89 (99%)	67 (76%)	21 (24%)	0	4
32	g	98/100 (98%)	75 (76%)	23 (24%)	1	5
33	h	109/110 (99%)	90 (83%)	19 (17%)	2	12
34	i	86/89 (97%)	73 (85%)	13 (15%)	3	19
35	j	73/80 (91%)	57 (78%)	16 (22%)	1	6
36	k	64/65 (98%)	51 (80%)	13 (20%)	1	8
37	l	47/48 (98%)	37 (79%)	10 (21%)	1	7
38	m	48/116 (41%)	37 (77%)	11 (23%)	1	5
39	o	92/94 (98%)	71 (77%)	21 (23%)	1	5
40	p	74/75 (99%)	60 (81%)	14 (19%)	1	9
41	r	109/121 (90%)	88 (81%)	21 (19%)	1	9
42	s	166/258 (64%)	148 (89%)	18 (11%)	6	32
43	t	136/137 (99%)	120 (88%)	16 (12%)	5	28
44	v	116/445 (26%)	99 (85%)	17 (15%)	3	20
45	0	34/1611 (2%)	30 (88%)	4 (12%)	5	28
45	w	11/1611 (1%)	9 (82%)	2 (18%)	1	10
45	z	119/1611 (7%)	103 (87%)	16 (13%)	4	23
47	1	13/79 (16%)	11 (85%)	2 (15%)	2	18
All	All	6105/11841 (52%)	5029 (82%)	1076 (18%)	4	12

All (1076) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	VAL
1	A	5	ILE
1	A	6	ARG
1	A	17	ARG
1	A	64	ARG
1	A	70	LYS
1	A	82	ILE
1	A	96	LEU
1	A	97	ASN
1	A	102	LEU
1	A	122	ASP
1	A	123	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	128	ARG
1	A	142	GLU
1	A	147	ARG
1	A	148	VAL
1	A	158	ILE
1	A	162	ASN
1	A	163	ARG
1	A	175	ILE
1	A	192	LYS
1	A	193	ARG
1	A	200	ARG
1	A	205	ASN
1	A	207	VAL
1	A	218	HIS
1	A	221	LYS
1	A	226	ARG
1	A	227	ARG
1	A	233	ARG
1	A	245	ARG
2	B	10	ARG
2	B	28	LYS
2	B	41	VAL
2	B	53	MET
2	B	56	ILE
2	B	60	VAL
2	B	62	ARG
2	B	66	LYS
2	B	94	GLU
2	B	95	THR
2	B	99	LEU
2	B	101	THR
2	B	103	LYS
2	B	116	ARG
2	B	120	LYS
2	B	135	LYS
2	B	138	GLN
2	B	167	GLN
2	B	175	GLN
2	B	181	MET
2	B	201	LEU
2	B	203	GLN
2	B	213	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	223	THR
2	B	228	TYR
2	B	231	VAL
2	B	233	SER
2	B	234	ARG
2	B	237	THR
2	B	240	LEU
2	B	248	LEU
2	B	258	HIS
2	B	261	ARG
2	B	262	VAL
2	B	264	PHE
2	B	279	GLU
2	B	293	ILE
2	B	305	THR
2	B	309	LEU
2	B	314	ILE
2	B	328	ASN
2	B	329	ASP
2	B	344	VAL
2	B	349	LYS
2	B	351	LEU
2	B	352	LEU
2	B	356	LYS
2	B	357	ARG
2	B	379	PHE
2	B	383	GLU
3	C	14	LYS
3	C	20	LYS
3	C	23	THR
3	C	24	LEU
3	C	38	ASN
3	C	44	LEU
3	C	48	ASN
3	C	49	ARG
3	C	55	SER
3	C	57	LEU
3	C	61	GLN
3	C	65	GLU
3	C	71	ARG
3	C	76	ILE
3	C	80	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	95	MET
3	C	97	ARG
3	C	101	MET
3	C	107	THR
3	C	114	ARG
3	C	117	THR
3	C	122	TYR
3	C	126	SER
3	C	140	LYS
3	C	144	ILE
3	C	147	VAL
3	C	150	LEU
3	C	155	GLU
3	C	163	LYS
3	C	173	LYS
3	C	175	LYS
3	C	188	ARG
3	C	189	MET
3	C	193	LYS
3	C	201	ARG
3	C	204	ARG
3	C	212	ASN
3	C	219	LYS
3	C	222	ARG
3	C	232	VAL
3	C	237	ILE
3	C	258	ARG
3	C	261	ASP
3	C	262	GLU
3	C	267	TRP
3	C	281	MET
3	C	284	MET
3	C	288	ASP
3	C	289	LEU
3	C	290	SER
3	C	294	LYS
3	C	307	LYS
3	C	309	ILE
3	C	312	ARG
3	C	317	ASN
3	C	321	ASN
3	C	333	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	335	MET
3	C	336	ARG
3	C	341	LEU
3	C	342	ARG
3	C	345	ARG
4	D	4	VAL
4	D	23	ARG
4	D	33	ARG
4	D	37	VAL
4	D	42	ASN
4	D	50	ARG
4	D	51	MET
4	D	66	TYR
4	D	73	MET
4	D	89	LYS
4	D	94	ASN
4	D	104	LEU
4	D	110	LEU
4	D	111	ASN
4	D	118	ILE
4	D	124	GLU
4	D	128	ASP
4	D	144	CYS
4	D	160	PHE
4	D	164	LYS
4	D	179	ARG
4	D	190	PHE
4	D	196	ARG
4	D	202	GLN
4	D	221	LYS
4	D	225	GLN
4	D	229	ASN
4	D	248	ARG
4	D	254	GLU
4	D	256	LYS
4	D	258	LYS
4	D	259	LYS
4	D	260	GLU
4	D	264	LYS
4	D	268	ARG
4	D	270	LYS
4	D	272	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	278	ASP
4	D	289	ARG
4	D	293	ARG
5	E	46	LEU
5	E	52	ARG
5	E	55	ARG
5	E	101	ARG
5	E	105	LEU
5	E	108	MET
5	E	115	GLU
5	E	134	ARG
5	E	136	LEU
5	E	137	ARG
5	E	144	THR
5	E	148	ILE
5	E	158	VAL
5	E	162	LYS
5	E	163	GLN
5	E	171	VAL
5	E	179	ARG
5	E	186	HIS
5	E	206	LYS
5	E	210	ASP
5	E	212	TYR
5	E	218	LEU
5	E	219	ARG
5	E	228	ILE
5	E	230	ASP
5	E	233	LYS
5	E	236	TYR
5	E	240	GLU
5	E	242	ARG
5	E	250	ASP
5	E	254	LEU
5	E	256	ARG
5	E	268	ARG
5	E	273	LEU
5	E	277	ILE
5	E	282	LEU
5	E	284	PHE
6	F	33	LYS
6	F	37	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	F	38	LYS
6	F	41	GLN
6	F	44	LEU
6	F	49	ARG
6	F	51	LEU
6	F	65	GLN
6	F	68	ARG
6	F	69	THR
6	F	70	GLU
6	F	72	ARG
6	F	82	ASN
6	F	90	LYS
6	F	91	LEU
6	F	96	ARG
6	F	98	ARG
6	F	100	ILE
6	F	101	ASN
6	F	104	SER
6	F	115	ARG
6	F	121	ASN
6	F	127	LEU
6	F	136	ARG
6	F	137	ILE
6	F	154	GLU
6	F	181	LEU
6	F	189	MET
6	F	190	GLU
6	F	192	LEU
6	F	201	LYS
6	F	202	ARG
6	F	214	LYS
6	F	234	ASP
6	F	238	ARG
6	F	241	GLN
6	F	247	ARG
6	F	248	ARG
7	G	28	VAL
7	G	29	ASN
7	G	31	LEU
7	G	46	GLN
7	G	50	ASP
7	G	59	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	G	62	ARG
7	G	67	ARG
7	G	71	TYR
7	G	73	ARG
7	G	76	VAL
7	G	81	ASN
7	G	88	ASP
7	G	90	GLN
7	G	101	LYS
7	G	108	GLN
7	G	110	LYS
7	G	121	LYS
7	G	131	LYS
7	G	148	GLU
7	G	150	LYS
7	G	151	LYS
7	G	154	LEU
7	G	170	LEU
7	G	173	LEU
7	G	175	ARG
7	G	177	MET
7	G	182	CYS
7	G	189	ARG
7	G	210	GLU
7	G	217	LYS
7	G	219	VAL
7	G	220	GLU
7	G	223	ARG
7	G	227	ASN
7	G	229	ARG
7	G	240	ASN
7	G	250	ILE
8	H	1	MET
8	H	19	THR
8	H	20	LEU
8	H	25	VAL
8	H	26	ILE
8	H	28	LYS
8	H	33	THR
8	H	40	HIS
8	H	41	ILE
8	H	42	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	H	52	LYS
8	H	54	ARG
8	H	57	VAL
8	H	59	LYS
8	H	66	GLU
8	H	67	LEU
8	H	72	THR
8	H	74	CYS
8	H	78	GLN
8	H	82	LYS
8	H	92	MET
8	H	105	ILE
8	H	106	GLN
8	H	111	LEU
8	H	117	PHE
8	H	125	ARG
8	H	128	MET
8	H	129	ARG
8	H	141	LYS
8	H	162	GLN
8	H	168	LYS
8	H	173	ARG
8	H	177	ASP
8	H	188	GLN
9	I	8	CYS
9	I	9	TYR
9	I	13	LYS
9	I	23	CYS
9	I	36	LEU
9	I	39	LYS
9	I	40	LYS
9	I	48	LEU
9	I	55	ASP
9	I	61	SER
9	I	66	GLU
9	I	71	CYS
9	I	73	ASN
9	I	74	LYS
9	I	76	MET
9	I	79	SER
9	I	80	CYS
9	I	88	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	I	92	HIS
9	I	100	ASN
9	I	113	THR
9	I	116	ARG
9	I	125	THR
9	I	139	ARG
9	I	141	LYS
9	I	142	LEU
9	I	144	ASN
9	I	146	GLU
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	175	LYS
9	I	180	GLU
9	I	187	LYS
9	I	189	CYS
9	I	208	LYS
9	I	212	LEU
10	J	14	GLU
10	J	15	LEU
10	J	16	ARG
10	J	23	ASN
10	J	49	VAL
10	J	52	LYS
10	J	55	TYR
10	J	81	GLU
10	J	94	LEU
10	J	96	LYS
10	J	113	ILE
10	J	136	ARG
10	J	147	ARG
10	J	150	CYS
10	J	151	ILE
10	J	154	LYS
10	J	164	ARG
10	J	168	GLN
10	J	171	ASP
11	L	5	ARG
11	L	10	LEU
11	L	11	LYS
11	L	19	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	L	35	ARG
11	L	36	ARG
11	L	49	ARG
11	L	59	VAL
11	L	64	VAL
11	L	65	ARG
11	L	74	ARG
11	L	77	SER
11	L	79	GLU
11	L	88	LYS
11	L	92	ARG
11	L	94	ILE
11	L	99	ASP
11	L	103	ARG
11	L	107	THR
11	L	111	GLN
11	L	113	ASN
11	L	115	GLN
11	L	119	GLU
11	L	121	ARG
11	L	123	LYS
11	L	130	LYS
11	L	143	GLU
11	L	154	VAL
11	L	158	ARG
11	L	162	LYS
11	L	165	LYS
11	L	172	GLU
11	L	186	ARG
11	L	190	ARG
11	L	194	ILE
11	L	195	ARG
11	L	198	ARG
11	L	201	GLU
11	L	208	GLU
12	M	5	ARG
12	M	8	GLU
12	M	29	ASP
12	M	32	ASP
12	M	33	GLN
12	M	43	THR
12	M	47	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	M	56	GLN
12	M	57	LEU
12	M	59	ASP
12	M	62	LEU
12	M	96	GLU
12	M	98	ARG
12	M	105	THR
12	M	113	MET
12	M	116	ARG
12	M	119	ARG
12	M	121	ARG
12	M	127	VAL
12	M	130	LEU
12	M	137	LYS
13	N	9	GLU
13	N	26	ARG
13	N	32	GLN
13	N	36	LEU
13	N	43	THR
13	N	44	ARG
13	N	49	ARG
13	N	61	ILE
13	N	63	ARG
13	N	64	ILE
13	N	72	LYS
13	N	75	VAL
13	N	77	LYS
13	N	87	HIS
13	N	89	VAL
13	N	100	SER
13	N	108	ARG
13	N	123	GLU
13	N	128	LYS
13	N	138	PHE
13	N	162	ARG
13	N	169	ARG
13	N	174	LEU
13	N	180	PHE
13	N	182	HIS
13	N	189	ARG
13	N	193	ARG
13	N	196	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	N	198	LEU
14	O	22	ILE
14	O	27	VAL
14	O	36	VAL
14	O	37	ARG
14	O	49	ARG
14	O	60	LYS
14	O	67	SER
14	O	74	ARG
14	O	82	ARG
14	O	85	ARG
14	O	99	LEU
14	O	117	ARG
14	O	153	THR
14	O	160	ARG
14	O	165	LYS
14	O	175	MET
14	O	178	ARG
14	O	179	LYS
14	O	184	ASN
14	O	187	LYS
14	O	188	LYS
14	O	202	LEU
15	P	5	SER
15	P	18	ARG
15	P	24	VAL
15	P	25	HIS
15	P	30	ARG
15	P	41	ILE
15	P	54	GLN
15	P	57	CYS
15	P	64	ASN
15	P	69	ARG
15	P	80	GLN
15	P	86	LYS
15	P	91	LEU
15	P	99	GLU
15	P	100	SER
15	P	103	GLU
15	P	104	LEU
15	P	105	LYS
15	P	110	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	P	126	ARG
15	P	127	ARG
15	P	128	ARG
15	P	144	CYS
15	P	154	GLU
16	Q	5	ILE
16	Q	13	VAL
16	Q	31	LEU
16	Q	37	ARG
16	Q	39	THR
16	Q	63	LEU
16	Q	65	ARG
16	Q	68	ARG
16	Q	69	LYS
16	Q	75	ARG
16	Q	78	LYS
16	Q	79	THR
16	Q	88	ASP
16	Q	91	ARG
16	Q	93	GLN
16	Q	97	LYS
16	Q	103	LEU
16	Q	108	ARG
16	Q	112	ARG
16	Q	119	LYS
16	Q	120	ILE
16	Q	126	LEU
16	Q	158	THR
16	Q	168	ARG
16	Q	172	ARG
16	Q	187	LYS
17	R	10	LEU
17	R	15	LEU
17	R	37	SER
17	R	39	GLN
17	R	40	GLN
17	R	42	ARG
17	R	43	LYS
17	R	46	LYS
17	R	47	ASP
17	R	50	ILE
17	R	52	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	R	59	SER
17	R	64	ARG
17	R	70	ARG
17	R	74	ARG
17	R	75	HIS
17	R	89	MET
17	R	94	THR
17	R	98	ARG
17	R	99	MET
17	R	103	ARG
17	R	105	LEU
17	R	106	LEU
17	R	107	ARG
17	R	113	LYS
17	R	117	ARG
17	R	120	TYR
17	R	133	LYS
17	R	136	ARG
17	R	137	ILE
17	R	138	LEU
17	R	168	GLU
17	R	180	LYS
18	S	2	LYS
18	S	7	LEU
18	S	8	ARG
18	S	9	GLU
18	S	13	VAL
18	S	17	LEU
18	S	36	ASN
18	S	39	VAL
18	S	67	VAL
18	S	68	PHE
18	S	69	GLU
18	S	70	LYS
18	S	80	ILE
18	S	82	LEU
18	S	83	ARG
18	S	84	TYR
18	S	90	THR
18	S	91	HIS
18	S	92	ASN
18	S	94	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	S	95	ARG
18	S	100	LEU
18	S	102	THR
18	S	108	GLN
18	S	120	ARG
18	S	127	MET
18	S	147	ASP
18	S	149	LYS
18	S	156	HIS
18	S	159	LEU
18	S	174	THR
19	T	5	LYS
19	T	7	LYS
19	T	9	ARG
19	T	17	ARG
19	T	29	THR
19	T	30	TYR
19	T	31	MET
19	T	33	ILE
19	T	35	LYS
19	T	60	LYS
19	T	67	VAL
19	T	70	HIS
19	T	81	LYS
19	T	83	LYS
19	T	88	ARG
19	T	96	ILE
19	T	99	SER
19	T	113	ASP
19	T	117	LYS
19	T	118	GLU
19	T	121	GLU
19	T	131	GLN
19	T	139	HIS
19	T	142	ARG
19	T	143	THR
19	T	144	ASN
19	T	146	LYS
19	T	159	MET
20	U	22	THR
20	U	23	LEU
20	U	26	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
20	U	27	HIS
20	U	33	ILE
20	U	38	ASN
20	U	45	GLU
20	U	46	ARG
20	U	63	ILE
20	U	64	GLU
20	U	65	ARG
20	U	67	LYS
20	U	69	LYS
20	U	80	LYS
20	U	99	TRP
20	U	101	ARG
20	U	113	ARG
21	V	14	PHE
21	V	15	ARG
21	V	18	LEU
21	V	25	VAL
21	V	30	ASP
21	V	31	ASN
21	V	35	LYS
21	V	51	ARG
21	V	60	MET
21	V	61	VAL
21	V	82	ILE
21	V	91	LYS
21	V	109	LYS
21	V	115	SER
21	V	123	LYS
22	W	25	ASP
22	W	27	LYS
22	W	43	LYS
22	W	48	GLN
22	W	50	ASN
22	W	54	LEU
23	X	39	LYS
23	X	41	ARG
23	X	43	SER
23	X	52	LEU
23	X	59	LYS
23	X	62	ARG
23	X	93	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
23	X	94	ASN
23	X	102	VAL
23	X	111	GLN
23	X	116	LEU
23	X	119	ILE
23	X	129	ARG
23	X	145	ASP
23	X	149	VAL
23	X	152	LYS
24	Y	2	LYS
24	Y	3	PHE
24	Y	8	THR
24	Y	11	ARG
24	Y	27	ARG
24	Y	28	LYS
24	Y	38	LEU
24	Y	50	ARG
24	Y	55	VAL
24	Y	59	ARG
24	Y	65	GLN
24	Y	72	GLN
24	Y	74	TYR
24	Y	87	ARG
24	Y	104	VAL
24	Y	112	ASP
24	Y	115	ARG
24	Y	117	LYS
24	Y	126	ARG
24	Y	127	GLN
25	Z	21	ARG
25	Z	27	LYS
25	Z	42	LEU
25	Z	57	MET
25	Z	59	LYS
25	Z	60	LYS
25	Z	65	ARG
25	Z	83	THR
25	Z	88	ASP
25	Z	91	LEU
25	Z	93	LYS
25	Z	97	ASN
25	Z	99	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	Z	101	PHE
25	Z	112	ARG
25	Z	121	ARG
26	a	5	LEU
26	a	7	LYS
26	a	8	THR
26	a	10	LYS
26	a	24	LYS
26	a	42	ARG
26	a	52	TYR
26	a	58	MET
26	a	59	ARG
26	a	72	THR
26	a	73	VAL
26	a	77	LYS
26	a	82	VAL
26	a	84	GLU
26	a	87	ARG
26	a	122	VAL
26	a	147	VAL
27	b	22	LYS
27	b	25	ARG
27	b	27	GLN
27	b	28	ARG
27	b	30	GLU
27	b	36	ASP
27	b	39	PHE
27	b	43	MET
27	b	44	ARG
27	b	51	LYS
27	b	68	ARG
28	c	15	ASN
28	c	16	SER
28	c	28	VAL
28	c	37	MET
28	c	40	GLN
28	c	50	ASN
28	c	51	ASN
28	c	78	ASN
28	c	89	TYR
28	c	94	LEU
29	d	19	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
29	d	23	ARG
29	d	26	THR
29	d	28	ASN
29	d	31	LYS
29	d	38	PHE
29	d	46	LEU
29	d	48	GLU
29	d	56	GLU
29	d	57	MET
29	d	75	LYS
29	d	77	ILE
29	d	78	ARG
29	d	79	ASN
29	d	84	ILE
29	d	85	ARG
29	d	94	GLU
29	d	102	LEU
29	d	107	THR
29	d	117	LEU
30	e	4	LEU
30	e	13	VAL
30	e	16	ARG
30	e	19	LYS
30	e	21	ILE
30	e	22	ARG
30	e	32	LYS
30	e	46	ARG
30	e	47	ARG
30	e	48	ARG
30	e	50	LYS
30	e	58	ILE
30	e	64	LYS
30	e	76	LYS
30	e	77	PHE
30	e	78	LEU
30	e	81	ASN
30	e	83	LYS
30	e	85	LEU
30	e	86	GLU
30	e	93	LYS
30	e	102	ASN
30	e	104	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
30	e	106	LYS
30	e	107	ASN
30	e	117	GLN
30	e	118	LEU
30	e	122	VAL
30	e	123	THR
30	e	128	ARG
30	e	129	LEU
31	f	7	SER
31	f	14	TYR
31	f	16	ARG
31	f	19	ARG
31	f	21	GLN
31	f	29	LYS
31	f	36	ARG
31	f	38	GLU
31	f	40	GLU
31	f	46	ARG
31	f	52	LYS
31	f	60	PRO
31	f	63	LYS
31	f	64	PRO
31	f	69	VAL
31	f	84	VAL
31	f	100	ARG
31	f	101	ILE
31	f	103	VAL
31	f	106	TYR
31	f	110	ILE
32	g	3	GLN
32	g	5	LEU
32	g	11	LEU
32	g	14	ASN
32	g	15	THR
32	g	18	ASN
32	g	19	LYS
32	g	23	SER
32	g	28	ASN
32	g	43	LYS
32	g	54	ARG
32	g	60	ARG
32	g	64	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	g	66	ARG
32	g	73	HIS
32	g	74	VAL
32	g	76	ARG
32	g	88	ARG
32	g	90	ARG
32	g	93	ARG
32	g	105	LYS
32	g	112	GLN
32	g	115	LYS
33	h	7	ARG
33	h	10	ARG
33	h	14	LYS
33	h	19	LYS
33	h	28	LEU
33	h	46	LYS
33	h	51	ARG
33	h	59	THR
33	h	62	ASN
33	h	65	GLN
33	h	71	LYS
33	h	88	THR
33	h	89	ARG
33	h	97	LYS
33	h	98	HIS
33	h	117	ARG
33	h	118	LYS
33	h	121	VAL
33	h	122	LYS
34	i	4	ARG
34	i	18	THR
34	i	25	ARG
34	i	29	ARG
34	i	34	THR
34	i	36	HIS
34	i	53	TYR
34	i	66	ASP
34	i	84	LYS
34	i	85	ARG
34	i	86	LYS
34	i	87	ARG
34	i	103	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	j	3	LYS
35	j	10	LYS
35	j	15	THR
35	j	20	ARG
35	j	25	LYS
35	j	29	LEU
35	j	33	THR
35	j	46	LYS
35	j	55	ARG
35	j	61	THR
35	j	63	ARG
35	j	68	LYS
35	j	72	ARG
35	j	79	ARG
35	j	83	THR
35	j	87	LYS
36	k	11	PHE
36	k	14	THR
36	k	18	LYS
36	k	19	ASP
36	k	21	LYS
36	k	29	LYS
36	k	36	VAL
36	k	37	ARG
36	k	54	GLU
36	k	56	LEU
36	k	57	LYS
36	k	69	LEU
36	k	70	LYS
37	l	4	HIS
37	l	8	ARG
37	l	16	LYS
37	l	17	GLN
37	l	20	ASN
37	l	21	ARG
37	l	33	ASN
37	l	36	ARG
37	l	46	ARG
37	l	47	THR
38	m	79	GLU
38	m	82	LEU
38	m	85	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
38	m	90	ASN
38	m	92	ASP
38	m	97	ARG
38	m	104	HIS
38	m	106	ARG
38	m	111	ARG
38	m	114	LYS
38	m	119	ASN
39	o	9	ARG
39	o	17	LYS
39	o	18	HIS
39	o	24	THR
39	o	26	TYR
39	o	33	LEU
39	o	36	GLN
39	o	40	ARG
39	o	44	LYS
39	o	55	ILE
39	o	56	PHE
39	o	57	ARG
39	o	61	LYS
39	o	63	THR
39	o	69	ARG
39	o	78	ARG
39	o	81	ARG
39	o	82	MET
39	o	89	LYS
39	o	99	ARG
39	o	102	GLN
40	p	3	LYS
40	p	11	VAL
40	p	16	THR
40	p	24	LYS
40	p	33	GLN
40	p	47	MET
40	p	49	ARG
40	p	50	ARG
40	p	54	ILE
40	p	60	CYS
40	p	84	ARG
40	p	85	ARG
40	p	87	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
40	p	89	LEU
41	r	6	GLN
41	r	8	MET
41	r	12	ASN
41	r	13	CYS
41	r	14	SER
41	r	17	LEU
41	r	21	ASN
41	r	24	THR
41	r	26	SER
41	r	28	GLU
41	r	32	LEU
41	r	35	ARG
41	r	39	ARG
41	r	60	VAL
41	r	67	ARG
41	r	70	GLN
41	r	83	ASN
41	r	90	LEU
41	r	105	ASP
41	r	108	MET
41	r	118	LEU
42	s	11	SER
42	s	18	ILE
42	s	38	LYS
42	s	39	GLN
42	s	44	ARG
42	s	59	THR
42	s	65	ILE
42	s	68	HIS
42	s	83	ARG
42	s	91	THR
42	s	107	VAL
42	s	133	GLU
42	s	146	LYS
42	s	149	ARG
42	s	174	LEU
42	s	185	PHE
42	s	189	ILE
42	s	191	GLN
43	t	1	MET
43	t	14	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
43	t	22	VAL
43	t	40	LYS
43	t	41	LYS
43	t	44	ASP
43	t	95	GLN
43	t	96	LYS
43	t	104	ILE
43	t	106	PHE
43	t	107	ASP
43	t	108	GLU
43	t	114	ARG
43	t	119	ARG
43	t	123	ARG
43	t	141	CYS
44	v	316	GLU
44	v	324	ASP
44	v	334	LEU
44	v	337	LEU
44	v	341	GLN
44	v	342	GLU
44	v	350	LEU
44	v	355	LEU
44	v	372	GLN
44	v	373	ILE
44	v	384	GLU
44	v	405	HIS
44	v	407	THR
44	v	409	LEU
44	v	411	ARG
44	v	463	VAL
44	v	465	LEU
45	w	13	LEU
45	w	20	ARG
45	z	1563	LEU
45	z	1571	THR
45	z	1582	TRP
45	z	1595	ASP
45	z	1597	PHE
45	z	1629	ARG
45	z	1632	THR
45	z	1633	ARG
45	z	1649	ILE

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Mol	Chain	Res	Type
45	z	1656	TYR
45	z	1661	ILE
45	z	1668	ARG
45	z	1681	LEU
45	z	1695	MET
45	z	1706	ASP
45	z	1709	PHE
45	0	1734	CYS
45	0	1741	PHE
45	0	1755	LYS
45	0	1765	PHE
47	1	13	ARG
47	1	24	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	205	ASN
2	B	25	HIS
2	B	138	GLN
2	B	289	GLN
2	B	301	ASN
2	B	376	HIS
3	C	61	GLN
3	C	317	ASN
4	D	81	HIS
4	D	282	GLN
5	E	39	HIS
5	E	43	ASN
5	E	207	HIS
5	E	246	GLN
6	F	41	GLN
6	F	82	ASN
6	F	174	ASN
6	F	241	GLN
6	F	243	ASN
9	I	73	ASN
10	J	23	ASN
10	J	98	ASN
11	L	28	GLN
12	M	56	GLN

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Mol	Chain	Res	Type
12	M	83	ASN
13	N	32	GLN
13	N	181	HIS
13	N	182	HIS
14	O	5	GLN
14	O	42	ASN
14	O	72	HIS
14	O	96	GLN
14	O	199	HIS
15	P	34	GLN
15	P	40	HIS
15	P	64	ASN
15	P	80	GLN
16	Q	44	ASN
16	Q	188	ASN
18	S	36	ASN
19	T	98	HIS
19	T	144	ASN
20	U	95	ASN
23	X	105	ASN
25	Z	97	ASN
27	b	11	ASN
27	b	12	GLN
28	c	40	GLN
28	c	51	ASN
28	c	78	ASN
29	d	34	HIS
29	d	100	ASN
31	f	20	ASN
31	f	56	ASN
31	f	99	HIS
32	g	28	ASN
33	h	96	ASN
35	j	16	HIS
39	o	90	HIS
41	r	6	GLN
41	r	12	ASN
41	r	31	ASN
44	v	372	GLN

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
48	2	73/77 (94%)	31 (42%)	2 (2%)
49	5	3646/3664 (99%)	1364 (37%)	373 (10%)
50	7	119/120 (99%)	27 (22%)	1 (0%)
51	8	155/156 (99%)	50 (32%)	9 (5%)
All	All	3993/4017 (99%)	1472 (36%)	385 (9%)

All (1472) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
48	2	3	C
48	2	5	G
48	2	7	G
48	2	11	A
48	2	13	C
48	2	16	C
48	2	19	G
48	2	20	U
48	2	21	A
48	2	26	G
48	2	33	U
48	2	35	A
48	2	38	A
48	2	39	C
48	2	42	G
48	2	43	A
48	2	44	A
48	2	45	G
48	2	46	G
48	2	47	U
48	2	48	C
48	2	49	G
48	2	51	C
48	2	53	G
48	2	57	A
48	2	58	A
48	2	60	U
48	2	63	G
48	2	67	C
48	2	72	A
48	2	76	A
49	5	2	G
49	5	6	C
49	5	8	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	12	A
49	5	13	U
49	5	15	A
49	5	16	G
49	5	20	U
49	5	21	G
49	5	25	A
49	5	29	G
49	5	39	A
49	5	43	U
49	5	48	G
49	5	49	U
49	5	56	A
49	5	58	G
49	5	59	A
49	5	64	A
49	5	65	A
49	5	66	A
49	5	68	U
49	5	69	A
49	5	71	C
49	5	73	A
49	5	74	G
49	5	75	G
49	5	84	A
49	5	85	G
49	5	88	A
49	5	91	G
49	5	93	G
49	5	94	A
49	5	104	G
49	5	108	A
49	5	109	G
49	5	110	C
49	5	116	G
49	5	118	C
49	5	119	G
49	5	120	A
49	5	121	A
49	5	122	U
49	5	126	C
49	5	128	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	129	C
49	5	134	G
49	5	135	G
49	5	136	C
49	5	137	G
49	5	139	G
49	5	142	G
49	5	143	C
49	5	144	G
49	5	145	G
49	5	157	U
49	5	158	A
49	5	159	C
49	5	160	G
49	5	164	G
49	5	166	C
49	5	167	C
49	5	171	U
49	5	172	C
49	5	173	C
49	5	174	C
49	5	177	G
49	5	178	C
49	5	183	C
49	5	184	U
49	5	185	C
49	5	186	G
49	5	187	U
49	5	188	G
49	5	189	G
49	5	195	C
49	5	197	A
49	5	198	A
49	5	200	U
49	5	201	C
49	5	202	C
49	5	203	U
49	5	205	C
49	5	213	G
49	5	216	C
49	5	217	C
49	5	218	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	219	G
49	5	220	C
49	5	221	C
49	5	224	U
49	5	226	G
49	5	227	A
49	5	232	G
49	5	233	U
49	5	234	G
49	5	235	A
49	5	239	C
49	5	245	C
49	5	246	G
49	5	255	C
49	5	257	C
49	5	262	G
49	5	265	C
49	5	266	C
49	5	267	G
49	5	272	U
49	5	275	C
49	5	276	C
49	5	277	G
49	5	278	G
49	5	280	G
49	5	281	U
49	5	292	G
49	5	293	G
49	5	294	G
49	5	296	A
49	5	297	U
49	5	300	A
49	5	306	A
49	5	309	C
49	5	315	G
49	5	316	U
49	5	319	A
49	5	321	U
49	5	322	C
49	5	323	C
49	5	329	A
49	5	330	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	331	G
49	5	334	A
49	5	336	A
49	5	337	U
49	5	340	C
49	5	344	A
49	5	347	A
49	5	350	C
49	5	357	U
49	5	360	A
49	5	361	C
49	5	362	A
49	5	363	A
49	5	381	U
49	5	386	A
49	5	387	G
49	5	388	A
49	5	396	A
49	5	399	G
49	5	405	U
49	5	406	C
49	5	407	A
49	5	408	A
49	5	409	G
49	5	410	A
49	5	412	G
49	5	413	G
49	5	417	G
49	5	418	A
49	5	424	U
49	5	431	G
49	5	432	U
49	5	433	A
49	5	440	U
49	5	445	U
49	5	449	C
49	5	450	G
49	5	451	C
49	5	452	A
49	5	453	G
49	5	454	U
49	5	455	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	458	C
49	5	465	G
49	5	467	U
49	5	468	U
49	5	469	C
49	5	470	A
49	5	471	A
49	5	473	C
49	5	485	C
49	5	486	C
49	5	487	G
49	5	488	G
49	5	498	C
49	5	500	G
49	5	501	C
49	5	502	C
49	5	503	C
49	5	504	G
49	5	506	C
49	5	509	A
49	5	510	U
49	5	511	C
49	5	513	U
49	5	514	U
49	5	515	C
49	5	516	C
49	5	519	C
49	5	647	G
49	5	648	G
49	5	649	A
49	5	650	C
49	5	654	C
49	5	663	G
49	5	664	G
49	5	665	C
49	5	666	G
49	5	667	A
49	5	668	C
49	5	669	C
49	5	682	G
49	5	683	C
49	5	684	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	685	C
49	5	686	A
49	5	687	U
49	5	688	U
49	5	689	U
49	5	690	C
49	5	694	C
49	5	695	G
49	5	696	C
49	5	697	G
49	5	698	G
49	5	702	U
49	5	703	G
49	5	704	C
49	5	707	C
49	5	712	C
49	5	718	C
49	5	721	G
49	5	723	A
49	5	724	C
49	5	728	U
49	5	729	G
49	5	730	G
49	5	732	A
49	5	737	C
49	5	742	G
49	5	743	G
49	5	745	G
49	5	746	A
49	5	747	A
49	5	748	G
49	5	749	G
49	5	756	G
49	5	911	U
49	5	914	U
49	5	915	A
49	5	917	A
49	5	918	G
49	5	920	C
49	5	925	C
49	5	927	G
49	5	928	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	929	A
49	5	930	G
49	5	931	C
49	5	932	A
49	5	933	G
49	5	934	C
49	5	935	A
49	5	936	C
49	5	937	U
49	5	938	C
49	5	939	G
49	5	940	C
49	5	942	G
49	5	943	A
49	5	944	A
49	5	945	U
49	5	946	C
49	5	952	G
49	5	956	A
49	5	957	G
49	5	958	G
49	5	959	G
49	5	960	A
49	5	961	G
49	5	962	C
49	5	963	G
49	5	964	A
49	5	965	G
49	5	966	A
49	5	967	C
49	5	968	C
49	5	969	C
49	5	971	U
49	5	972	C
49	5	974	C
49	5	976	G
49	5	977	C
49	5	978	G
49	5	979	C
49	5	982	U
49	5	983	C
49	5	989	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	990	C
49	5	1051	G
49	5	1070	G
49	5	1072	C
49	5	1075	G
49	5	1076	C
49	5	1081	C
49	5	1177	U
49	5	1181	C
49	5	1193	C
49	5	1195	G
49	5	1204	C
49	5	1209	U
49	5	1210	C
49	5	1211	G
49	5	1212	G
49	5	1214	C
49	5	1215	C
49	5	1219	G
49	5	1221	G
49	5	1222	A
49	5	1233	G
49	5	1235	G
49	5	1236	C
49	5	1237	C
49	5	1238	A
49	5	1239	C
49	5	1240	G
49	5	1242	G
49	5	1243	C
49	5	1244	G
49	5	1245	C
49	5	1255	A
49	5	1256	G
49	5	1265	G
49	5	1266	G
49	5	1267	C
49	5	1268	G
49	5	1269	G
49	5	1270	A
49	5	1271	G
49	5	1272	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	1273	G
49	5	1274	A
49	5	1275	G
49	5	1277	G
49	5	1279	A
49	5	1280	C
49	5	1281	G
49	5	1284	G
49	5	1285	U
49	5	1286	C
49	5	1288	G
49	5	1292	C
49	5	1293	G
49	5	1294	A
49	5	1295	C
49	5	1296	G
49	5	1297	U
49	5	1300	G
49	5	1301	C
49	5	1304	C
49	5	1313	C
49	5	1318	C
49	5	1326	A
49	5	1329	G
49	5	1330	A
49	5	1337	A
49	5	1338	G
49	5	1347	G
49	5	1353	G
49	5	1354	A
49	5	1357	C
49	5	1358	G
49	5	1359	G
49	5	1360	G
49	5	1364	U
49	5	1365	C
49	5	1366	G
49	5	1367	C
49	5	1369	C
49	5	1370	G
49	5	1371	A
49	5	1372	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	1377	G
49	5	1378	C
49	5	1379	C
49	5	1380	G
49	5	1381	U
49	5	1385	G
49	5	1387	A
49	5	1394	G
49	5	1397	A
49	5	1398	A
49	5	1399	G
49	5	1406	G
49	5	1407	C
49	5	1408	G
49	5	1409	C
49	5	1410	U
49	5	1411	C
49	5	1415	G
49	5	1416	G
49	5	1420	A
49	5	1421	G
49	5	1425	G
49	5	1426	G
49	5	1428	U
49	5	1429	C
49	5	1432	G
49	5	1435	G
49	5	1436	C
49	5	1439	C
49	5	1440	U
49	5	1441	C
49	5	1445	U
49	5	1446	C
49	5	1448	G
49	5	1454	G
49	5	1455	G
49	5	1456	C
49	5	1457	G
49	5	1465	G
49	5	1468	C
49	5	1474	C
49	5	1475	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	1477	C
49	5	1478	C
49	5	1480	C
49	5	1482	G
49	5	1483	C
49	5	1484	G
49	5	1485	C
49	5	1486	C
49	5	1489	G
49	5	1493	G
49	5	1497	A
49	5	1498	G
49	5	1500	A
49	5	1501	C
49	5	1502	G
49	5	1504	G
49	5	1516	G
49	5	1518	A
49	5	1523	A
49	5	1524	A
49	5	1529	G
49	5	1530	G
49	5	1534	A
49	5	1535	C
49	5	1543	G
49	5	1547	A
49	5	1554	A
49	5	1559	G
49	5	1560	A
49	5	1563	A
49	5	1564	A
49	5	1566	C
49	5	1568	C
49	5	1569	U
49	5	1571	G
49	5	1578	U
49	5	1586	G
49	5	1591	U
49	5	1594	C
49	5	1596	U
49	5	1601	A
49	5	1602	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	1611	C
49	5	1612	G
49	5	1613	A
49	5	1624	G
49	5	1625	G
49	5	1631	A
49	5	1633	G
49	5	1634	A
49	5	1636	U
49	5	1637	A
49	5	1638	A
49	5	1641	G
49	5	1642	A
49	5	1643	A
49	5	1650	A
49	5	1654	G
49	5	1655	C
49	5	1656	U
49	5	1661	C
49	5	1670	G
49	5	1676	C
49	5	1677	U
49	5	1680	G
49	5	1684	A
49	5	1685	G
49	5	1687	U
49	5	1691	G
49	5	1692	C
49	5	1696	C
49	5	1697	G
49	5	1698	C
49	5	1699	A
49	5	1719	A
49	5	1720	C
49	5	1721	G
49	5	1724	G
49	5	1725	U
49	5	1727	U
49	5	1733	G
49	5	1734	G
49	5	1736	A
49	5	1742	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	1746	A
49	5	1750	G
49	5	1753	G
49	5	1754	U
49	5	1755	C
49	5	1756	U
49	5	1757	U
49	5	1758	G
49	5	1760	G
49	5	1761	G
49	5	1764	G
49	5	1767	A
49	5	1768	C
49	5	1770	A
49	5	1772	C
49	5	1775	A
49	5	1776	A
49	5	1777	C
49	5	1778	C
49	5	1779	U
49	5	1781	U
49	5	1785	C
49	5	1787	A
49	5	1790	U
49	5	1800	U
49	5	1803	G
49	5	1804	A
49	5	1805	A
49	5	1811	G
49	5	1812	C
49	5	1815	G
49	5	1817	U
49	5	1819	G
49	5	1820	C
49	5	1821	G
49	5	1822	U
49	5	1828	C
49	5	1830	G
49	5	1832	C
49	5	1833	G
49	5	1834	U
49	5	1835	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	1836	G
49	5	1843	A
49	5	1848	C
49	5	1851	G
49	5	1855	G
49	5	1869	G
49	5	1881	C
49	5	1882	U
49	5	1890	G
49	5	1897	A
49	5	1899	G
49	5	1900	C
49	5	1907	A
49	5	1910	G
49	5	1912	G
49	5	1913	C
49	5	1918	U
49	5	1919	G
49	5	1920	C
49	5	1921	C
49	5	1922	G
49	5	1923	A
49	5	1925	G
49	5	1929	A
49	5	1931	C
49	5	1932	A
49	5	1936	C
49	5	1938	C
49	5	1939	A
49	5	1941	A
49	5	1945	G
49	5	1947	U
49	5	1951	G
49	5	1956	A
49	5	1959	U
49	5	1961	G
49	5	1962	A
49	5	1964	A
49	5	1966	C
49	5	1969	G
49	5	1972	G
49	5	1975	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	1976	G
49	5	1977	C
49	5	1979	A
49	5	1980	U
49	5	1981	G
49	5	1983	A
49	5	1984	A
49	5	1985	G
49	5	1987	C
49	5	1988	G
49	5	1991	A
49	5	1992	U
49	5	1993	C
49	5	1995	G
49	5	1997	U
49	5	1998	A
49	5	2001	G
49	5	2002	A
49	5	2003	G
49	5	2004	U
49	5	2005	G
49	5	2007	G
49	5	2008	U
49	5	2009	A
49	5	2010	A
49	5	2011	C
49	5	2019	C
49	5	2023	C
49	5	2024	G
49	5	2025	A
49	5	2026	A
49	5	2033	A
49	5	2046	G
49	5	2047	A
49	5	2048	U
49	5	2052	G
49	5	2055	G
49	5	2056	G
49	5	2064	G
49	5	2069	A
49	5	2070	U
49	5	2077	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	2078	C
49	5	2079	G
49	5	2084	C
49	5	2085	G
49	5	2088	A
49	5	2089	G
49	5	2090	U
49	5	2091	C
49	5	2092	G
49	5	2093	A
49	5	2094	G
49	5	2095	A
49	5	2096	G
49	5	2097	U
49	5	2100	A
49	5	2102	G
49	5	2105	A
49	5	2107	C
49	5	2108	G
49	5	2109	G
49	5	2110	C
49	5	2111	G
49	5	2112	G
49	5	2113	G
49	5	2114	G
49	5	2115	G
49	5	2116	C
49	5	2117	G
49	5	2118	G
49	5	2119	C
49	5	2120	G
49	5	2121	C
49	5	2122	G
49	5	2123	C
49	5	2124	G
49	5	2125	C
49	5	2126	G
49	5	2127	C
49	5	2131	C
49	5	2247	C
49	5	2248	C
49	5	2250	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	2251	G
49	5	2252	G
49	5	2253	A
49	5	2254	G
49	5	2255	C
49	5	2256	C
49	5	2257	C
49	5	2258	C
49	5	2259	G
49	5	2260	C
49	5	2261	G
49	5	2263	A
49	5	2264	C
49	5	2265	G
49	5	2266	C
49	5	2267	U
49	5	2268	A
49	5	2269	C
49	5	2273	G
49	5	2275	G
49	5	2279	A
49	5	2281	U
49	5	2283	G
49	5	2289	C
49	5	2295	C
49	5	2297	G
49	5	2298	U
49	5	2300	A
49	5	2301	G
49	5	2312	U
49	5	2313	A
49	5	2314	G
49	5	2315	G
49	5	2319	C
49	5	2321	G
49	5	2322	G
49	5	2331	G
49	5	2333	G
49	5	2335	C
49	5	2337	C
49	5	2340	C
49	5	2342	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	2348	G
49	5	2351	C
49	5	2357	G
49	5	2360	A
49	5	2362	U
49	5	2364	G
49	5	2369	U
49	5	2370	A
49	5	2378	G
49	5	2382	A
49	5	2389	A
49	5	2390	G
49	5	2391	G
49	5	2395	A
49	5	2396	A
49	5	2398	U
49	5	2399	G
49	5	2401	A
49	5	2402	G
49	5	2404	A
49	5	2408	U
49	5	2417	A
49	5	2422	C
49	5	2425	U
49	5	2426	U
49	5	2428	A
49	5	2432	U
49	5	2433	G
49	5	2434	G
49	5	2440	U
49	5	2441	C
49	5	2443	G
49	5	2444	U
49	5	2445	C
49	5	2450	G
49	5	2458	C
49	5	2467	U
49	5	2469	C
49	5	2471	G
49	5	2474	G
49	5	2475	G
49	5	2476	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	2488	C
49	5	2489	C
49	5	2490	U
49	5	2491	C
49	5	2503	G
49	5	2504	C
49	5	2505	C
49	5	2506	G
49	5	2507	A
49	5	2508	U
49	5	2511	A
49	5	2512	A
49	5	2513	A
49	5	2514	G
49	5	2517	A
49	5	2518	G
49	5	2526	C
49	5	2527	A
49	5	2529	A
49	5	2530	U
49	5	2537	A
49	5	2538	U
49	5	2544	G
49	5	2546	G
49	5	2547	G
49	5	2549	G
49	5	2551	A
49	5	2553	A
49	5	2554	U
49	5	2555	G
49	5	2560	C
49	5	2563	C
49	5	2566	G
49	5	2571	C
49	5	2572	C
49	5	2577	C
49	5	2583	C
49	5	2586	G
49	5	2587	A
49	5	2588	C
49	5	2589	C
49	5	2601	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	2602	G
49	5	2611	A
49	5	2618	G
49	5	2620	G
49	5	2623	A
49	5	2627	C
49	5	2628	U
49	5	2630	U
49	5	2638	G
49	5	2640	G
49	5	2647	A
49	5	2661	U
49	5	2662	G
49	5	2663	G
49	5	2666	U
49	5	2670	C
49	5	2673	G
49	5	2675	G
49	5	2684	C
49	5	2686	G
49	5	2687	U
49	5	2689	C
49	5	2695	A
49	5	2696	A
49	5	2704	C
49	5	2708	U
49	5	2710	C
49	5	2711	G
49	5	2712	G
49	5	2713	C
49	5	2714	G
49	5	2716	C
49	5	2725	A
49	5	2726	G
49	5	2737	C
49	5	2740	U
49	5	2743	A
49	5	2744	A
49	5	2747	U
49	5	2752	G
49	5	2753	G
49	5	2754	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	2755	A
49	5	2756	G
49	5	2760	G
49	5	2761	U
49	5	2762	G
49	5	2764	A
49	5	2766	A
49	5	2767	U
49	5	2768	C
49	5	2769	U
49	5	2770	C
49	5	2787	A
49	5	2788	U
49	5	2789	A
49	5	2790	U
49	5	2793	G
49	5	2794	C
49	5	2796	G
49	5	2797	C
49	5	2798	A
49	5	2799	G
49	5	2806	A
49	5	2807	A
49	5	2813	A
49	5	2814	C
49	5	2815	A
49	5	2825	A
49	5	2826	U
49	5	2827	G
49	5	2828	U
49	5	2829	U
49	5	2833	A
49	5	2834	C
49	5	2835	A
49	5	2838	G
49	5	2839	U
49	5	2841	G
49	5	2842	G
49	5	2844	A
49	5	2852	U
49	5	2854	G
49	5	2855	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	2858	A
49	5	2859	G
49	5	2860	C
49	5	2863	G
49	5	2864	A
49	5	2867	C
49	5	2869	U
49	5	2874	U
49	5	2897	G
49	5	2898	G
49	5	2900	U
49	5	2904	U
49	5	2905	C
49	5	2910	G
49	5	3591	C
49	5	3594	C
49	5	3596	A
49	5	3597	G
49	5	3604	A
49	5	3605	C
49	5	3606	U
49	5	3614	G
49	5	3615	G
49	5	3616	U
49	5	3617	G
49	5	3625	G
49	5	3626	G
49	5	3627	G
49	5	3635	A
49	5	3643	A
49	5	3644	U
49	5	3648	A
49	5	3653	A
49	5	3657	U
49	5	3659	G
49	5	3660	C
49	5	3662	A
49	5	3663	A
49	5	3664	G
49	5	3667	C
49	5	3671	G
49	5	3672	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	3673	C
49	5	3674	G
49	5	3675	G
49	5	3679	U
49	5	3680	U
49	5	3681	G
49	5	3682	A
49	5	3696	C
49	5	3698	G
49	5	3701	C
49	5	3709	U
49	5	3710	G
49	5	3711	A
49	5	3712	A
49	5	3713	U
49	5	3714	G
49	5	3726	A
49	5	3727	A
49	5	3728	A
49	5	3729	U
49	5	3736	A
49	5	3738	G
49	5	3739	C
49	5	3743	G
49	5	3744	G
49	5	3745	U
49	5	3748	A
49	5	3750	G
49	5	3753	G
49	5	3756	A
49	5	3759	A
49	5	3765	G
49	5	3770	U
49	5	3773	U
49	5	3774	A
49	5	3776	G
49	5	3777	G
49	5	3784	A
49	5	3785	A
49	5	3786	U
49	5	3787	G
49	5	3791	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	3795	A
49	5	3799	A
49	5	3810	C
49	5	3811	G
49	5	3814	U
49	5	3817	A
49	5	3819	G
49	5	3822	U
49	5	3824	A
49	5	3831	U
49	5	3838	U
49	5	3839	G
49	5	3840	U
49	5	3851	U
49	5	3859	G
49	5	3867	A
49	5	3868	G
49	5	3869	C
49	5	3870	C
49	5	3871	A
49	5	3876	A
49	5	3877	A
49	5	3878	C
49	5	3879	G
49	5	3889	G
49	5	3892	U
49	5	3897	G
49	5	3898	G
49	5	3900	G
49	5	3901	A
49	5	3905	A
49	5	3906	A
49	5	3907	G
49	5	3912	U
49	5	3913	G
49	5	3914	U
49	5	3915	U
49	5	3916	G
49	5	3917	A
49	5	3923	A
49	5	3925	U
49	5	3926	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	3927	U
49	5	3932	U
49	5	3938	G
49	5	3939	G
49	5	3943	A
49	5	4069	U
49	5	4070	U
49	5	4073	A
49	5	4076	G
49	5	4084	G
49	5	4085	A
49	5	4086	G
49	5	4087	G
49	5	4088	C
49	5	4089	G
49	5	4091	G
49	5	4092	G
49	5	4093	G
49	5	4094	G
49	5	4097	G
49	5	4104	G
49	5	4105	A
49	5	4107	G
49	5	4114	C
49	5	4115	G
49	5	4116	C
49	5	4117	U
49	5	4118	U
49	5	4119	C
49	5	4120	U
49	5	4121	G
49	5	4122	G
49	5	4123	C
49	5	4125	C
49	5	4126	C
49	5	4127	A
49	5	4140	C
49	5	4143	G
49	5	4144	C
49	5	4145	C
49	5	4149	C
49	5	4151	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	4161	G
49	5	4164	C
49	5	4166	G
49	5	4171	C
49	5	4180	G
49	5	4182	G
49	5	4183	G
49	5	4184	G
49	5	4191	G
49	5	4195	G
49	5	4197	G
49	5	4203	A
49	5	4205	A
49	5	4206	C
49	5	4213	A
49	5	4214	A
49	5	4216	G
49	5	4217	G
49	5	4218	U
49	5	4219	A
49	5	4225	G
49	5	4228	G
49	5	4229	U
49	5	4232	U
49	5	4233	A
49	5	4235	G
49	5	4236	G
49	5	4237	C
49	5	4241	C
49	5	4249	G
49	5	4251	A
49	5	4254	G
49	5	4255	A
49	5	4267	G
49	5	4268	A
49	5	4271	A
49	5	4273	A
49	5	4274	A
49	5	4282	A
49	5	4286	C
49	5	4290	U
49	5	4291	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	4297	G
49	5	4305	G
49	5	4306	U
49	5	4313	A
49	5	4314	C
49	5	4317	A
49	5	4318	C
49	5	4323	A
49	5	4329	G
49	5	4330	G
49	5	4332	C
49	5	4335	C
49	5	4336	A
49	5	4337	C
49	5	4339	A
49	5	4349	C
49	5	4350	C
49	5	4354	U
49	5	4355	G
49	5	4359	U
49	5	4360	U
49	5	4367	G
49	5	4368	G
49	5	4374	U
49	5	4375	C
49	5	4376	A
49	5	4377	G
49	5	4378	A
49	5	4379	A
49	5	4387	C
49	5	4391	G
49	5	4394	A
49	5	4395	U
49	5	4398	C
49	5	4401	G
49	5	4419	U
49	5	4420	U
49	5	4422	A
49	5	4426	C
49	5	4433	G
49	5	4437	U
49	5	4438	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	4439	U
49	5	4441	A
49	5	4444	C
49	5	4448	G
49	5	4449	A
49	5	4450	U
49	5	4451	G
49	5	4452	U
49	5	4453	C
49	5	4464	A
49	5	4465	U
49	5	4466	C
49	5	4467	A
49	5	4472	G
49	5	4473	A
49	5	4475	G
49	5	4476	C
49	5	4481	U
49	5	4482	U
49	5	4484	A
49	5	4487	A
49	5	4488	A
49	5	4489	G
49	5	4490	C
49	5	4491	G
49	5	4497	U
49	5	4500	U
49	5	4511	A
49	5	4512	U
49	5	4513	A
49	5	4518	A
49	5	4519	C
49	5	4522	G
49	5	4523	A
49	5	4524	G
49	5	4528	G
49	5	4529	G
49	5	4530	U
49	5	4531	U
49	5	4532	U
49	5	4534	G
49	5	4537	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	4548	A
49	5	4549	G
49	5	4550	G
49	5	4552	U
49	5	4554	G
49	5	4555	U
49	5	4559	A
49	5	4560	C
49	5	4569	U
49	5	4570	G
49	5	4573	G
49	5	4575	G
49	5	4576	U
49	5	4577	U
49	5	4584	A
49	5	4585	U
49	5	4586	G
49	5	4589	A
49	5	4590	A
49	5	4605	A
49	5	4606	G
49	5	4608	G
49	5	4617	G
49	5	4623	G
49	5	4624	A
49	5	4629	U
49	5	4636	U
49	5	4637	G
49	5	4641	U
49	5	4646	U
49	5	4647	G
49	5	4648	A
49	5	4652	G
49	5	4656	A
49	5	4657	U
49	5	4661	G
49	5	4670	C
49	5	4671	C
49	5	4672	A
49	5	4677	U
49	5	4678	G
49	5	4687	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	4693	C
49	5	4694	G
49	5	4695	C
49	5	4700	A
49	5	4701	A
49	5	4703	U
49	5	4707	A
49	5	4709	U
49	5	4719	G
49	5	4720	C
49	5	4729	A
49	5	4730	C
49	5	4731	G
49	5	4732	G
49	5	4733	C
49	5	4734	A
49	5	4737	G
49	5	4741	C
49	5	4745	G
49	5	4746	C
49	5	4749	C
49	5	4750	G
49	5	4751	G
49	5	4752	U
49	5	4753	U
49	5	4756	C
49	5	4757	C
49	5	4758	U
49	5	4760	G
49	5	4763	U
49	5	4764	A
49	5	4770	U
49	5	4771	C
49	5	4774	C
49	5	4860	G
49	5	4865	C
49	5	4869	U
49	5	4871	C
49	5	4872	G
49	5	4873	G
49	5	4874	A
49	5	4875	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	4876	U
49	5	4877	G
49	5	4878	C
49	5	4881	U
49	5	4882	U
49	5	4883	C
49	5	4884	G
49	5	4885	U
49	5	4886	C
49	5	4888	U
49	5	4889	G
49	5	4890	G
49	5	4891	G
49	5	4893	A
49	5	4895	C
49	5	4896	G
49	5	4898	G
49	5	4900	C
49	5	4901	G
49	5	4903	G
49	5	4904	G
49	5	4906	C
49	5	4910	G
49	5	4911	A
49	5	4912	G
49	5	4913	G
49	5	4924	C
49	5	4926	C
49	5	4927	G
49	5	4929	C
49	5	4930	C
49	5	4932	U
49	5	4933	C
49	5	4934	A
49	5	4935	C
49	5	4936	G
49	5	4938	A
49	5	4942	C
49	5	4945	G
49	5	4946	U
49	5	4947	U
49	5	4948	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	4949	G
49	5	4950	U
49	5	4951	G
49	5	4952	G
49	5	4959	U
49	5	4960	G
49	5	4961	G
49	5	4964	C
49	5	4965	U
49	5	4966	A
49	5	4967	A
49	5	4975	G
49	5	4976	U
49	5	4980	C
49	5	4981	G
49	5	4985	U
49	5	4988	U
49	5	4989	U
49	5	4990	C
49	5	4991	U
49	5	4992	G
49	5	4993	G
49	5	4999	G
49	5	5002	U
49	5	5004	C
49	5	5005	G
49	5	5006	U
49	5	5007	A
49	5	5011	A
49	5	5013	C
49	5	5014	A
49	5	5016	A
49	5	5017	G
49	5	5018	C
49	5	5023	C
49	5	5026	U
49	5	5027	C
49	5	5028	G
49	5	5029	C
49	5	5031	G
49	5	5033	G
49	5	5035	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	5039	U
49	5	5041	G
49	5	5042	A
49	5	5045	G
49	5	5046	U
49	5	5047	C
49	5	5050	C
49	5	5052	C
49	5	5053	U
49	5	5054	C
49	5	5056	A
49	5	5058	A
49	5	5060	A
49	5	5061	A
49	5	5062	G
49	5	5063	G
49	5	5066	U
50	7	3	C
50	7	7	G
50	7	11	A
50	7	21	G
50	7	22	A
50	7	25	G
50	7	30	C
50	7	33	U
50	7	40	U
50	7	42	A
50	7	51	G
50	7	53	U
50	7	54	A
50	7	60	G
50	7	64	G
50	7	65	G
50	7	74	A
50	7	80	U
50	7	89	G
50	7	97	G
50	7	98	G
50	7	99	G
50	7	100	A
50	7	106	G
50	7	110	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	7	112	U
50	7	120	U
51	8	2	G
51	8	3	A
51	8	22	U
51	8	23	C
51	8	32	C
51	8	34	U
51	8	35	C
51	8	38	U
51	8	50	C
51	8	52	A
51	8	55	U
51	8	59	A
51	8	61	A
51	8	62	A
51	8	63	U
51	8	71	A
51	8	75	G
51	8	80	A
51	8	81	C
51	8	82	A
51	8	83	C
51	8	84	A
51	8	85	U
51	8	86	U
51	8	87	G
51	8	94	G
51	8	95	A
51	8	103	A
51	8	104	A
51	8	105	C
51	8	107	C
51	8	109	C
51	8	110	U
51	8	111	U
51	8	112	G
51	8	113	C
51	8	114	G
51	8	116	C
51	8	120	G
51	8	121	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	8	122	G
51	8	123	U
51	8	124	U
51	8	125	C
51	8	126	C
51	8	127	U
51	8	137	A
51	8	150	C
51	8	153	C
51	8	156	U

All (385) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	2	15	G
48	2	60	U
49	5	1	C
49	5	12	A
49	5	20	U
49	5	42	A
49	5	43	U
49	5	48	G
49	5	58	G
49	5	64	A
49	5	65	A
49	5	72	C
49	5	84	A
49	5	119	G
49	5	120	A
49	5	125	C
49	5	134	G
49	5	136	C
49	5	143	C
49	5	159	C
49	5	170	C
49	5	183	C
49	5	186	G
49	5	187	U
49	5	215	C
49	5	216	C
49	5	218	A
49	5	219	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	224	U
49	5	226	G
49	5	234	G
49	5	245	C
49	5	256	G
49	5	265	C
49	5	266	C
49	5	275	C
49	5	296	A
49	5	315	G
49	5	316	U
49	5	333	U
49	5	352	G
49	5	361	C
49	5	385	A
49	5	387	G
49	5	406	C
49	5	409	G
49	5	417	G
49	5	451	C
49	5	454	U
49	5	485	C
49	5	486	C
49	5	497	G
49	5	505	G
49	5	514	U
49	5	648	G
49	5	655	C
49	5	664	G
49	5	668	C
49	5	684	G
49	5	693	C
49	5	713	C
49	5	728	U
49	5	729	G
49	5	733	A
49	5	746	A
49	5	917	A
49	5	927	G
49	5	928	C
49	5	930	G
49	5	931	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	932	A
49	5	935	A
49	5	936	C
49	5	943	A
49	5	956	A
49	5	957	G
49	5	958	G
49	5	961	G
49	5	965	G
49	5	968	C
49	5	977	C
49	5	978	G
49	5	979	C
49	5	989	U
49	5	1067	G
49	5	1068	G
49	5	1070	G
49	5	1076	C
49	5	1210	C
49	5	1211	G
49	5	1214	C
49	5	1216	C
49	5	1217	G
49	5	1232	G
49	5	1236	C
49	5	1238	A
49	5	1239	C
49	5	1241	C
49	5	1243	C
49	5	1264	C
49	5	1266	G
49	5	1279	A
49	5	1280	C
49	5	1292	C
49	5	1293	G
49	5	1296	G
49	5	1313	C
49	5	1324	A
49	5	1329	G
49	5	1354	A
49	5	1357	C
49	5	1358	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	1359	G
49	5	1365	C
49	5	1368	A
49	5	1370	G
49	5	1371	A
49	5	1379	C
49	5	1380	G
49	5	1387	A
49	5	1397	A
49	5	1398	A
49	5	1407	C
49	5	1409	C
49	5	1410	U
49	5	1419	G
49	5	1420	A
49	5	1435	G
49	5	1440	U
49	5	1445	U
49	5	1455	G
49	5	1474	C
49	5	1477	C
49	5	1480	C
49	5	1481	C
49	5	1482	G
49	5	1485	C
49	5	1488	G
49	5	1500	A
49	5	1502	G
49	5	1523	A
49	5	1533	A
49	5	1596	U
49	5	1597	G
49	5	1601	A
49	5	1611	C
49	5	1633	G
49	5	1642	A
49	5	1650	A
49	5	1654	G
49	5	1696	C
49	5	1697	G
49	5	1724	G
49	5	1733	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	1741	G
49	5	1756	U
49	5	1775	A
49	5	1804	A
49	5	1815	G
49	5	1818	G
49	5	1819	G
49	5	1835	G
49	5	1898	C
49	5	1919	G
49	5	1920	C
49	5	1921	C
49	5	1928	C
49	5	1938	C
49	5	1960	A
49	5	1974	U
49	5	1975	G
49	5	1980	U
49	5	1983	A
49	5	1990	A
49	5	2002	A
49	5	2009	A
49	5	2025	A
49	5	2046	G
49	5	2068	C
49	5	2075	G
49	5	2083	C
49	5	2084	C
49	5	2089	G
49	5	2093	A
49	5	2096	G
49	5	2107	C
49	5	2111	G
49	5	2114	G
49	5	2116	C
49	5	2119	C
49	5	2122	G
49	5	2123	C
49	5	2126	G
49	5	2246	C
49	5	2251	G
49	5	2256	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	2257	C
49	5	2260	C
49	5	2262	G
49	5	2264	C
49	5	2265	G
49	5	2266	C
49	5	2267	U
49	5	2268	A
49	5	2269	C
49	5	2272	C
49	5	2278	G
49	5	2280	G
49	5	2289	C
49	5	2300	A
49	5	2305	U
49	5	2313	A
49	5	2331	G
49	5	2347	A
49	5	2348	G
49	5	2361	G
49	5	2389	A
49	5	2396	A
49	5	2398	U
49	5	2407	G
49	5	2443	G
49	5	2467	U
49	5	2468	U
49	5	2474	G
49	5	2475	G
49	5	2487	G
49	5	2490	U
49	5	2502	G
49	5	2506	G
49	5	2511	A
49	5	2512	A
49	5	2513	A
49	5	2517	A
49	5	2529	A
49	5	2546	G
49	5	2553	A
49	5	2554	U
49	5	2587	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	2588	C
49	5	2618	G
49	5	2661	U
49	5	2666	U
49	5	2673	G
49	5	2695	A
49	5	2711	G
49	5	2752	G
49	5	2754	G
49	5	2760	G
49	5	2761	U
49	5	2768	C
49	5	2769	U
49	5	2782	U
49	5	2788	U
49	5	2795	A
49	5	2796	G
49	5	2806	A
49	5	2825	A
49	5	2826	U
49	5	2827	G
49	5	2833	A
49	5	2857	A
49	5	2859	G
49	5	3593	C
49	5	3615	G
49	5	3625	G
49	5	3662	A
49	5	3663	A
49	5	3672	G
49	5	3673	C
49	5	3679	U
49	5	3697	U
49	5	3712	A
49	5	3726	A
49	5	3735	G
49	5	3773	U
49	5	3776	G
49	5	3783	A
49	5	3784	A
49	5	3786	U
49	5	3790	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	3791	C
49	5	3809	G
49	5	3811	G
49	5	3839	G
49	5	3876	A
49	5	3878	C
49	5	3888	G
49	5	3904	G
49	5	3905	A
49	5	3922	G
49	5	3938	G
49	5	4069	U
49	5	4075	U
49	5	4084	G
49	5	4086	G
49	5	4115	G
49	5	4117	U
49	5	4119	C
49	5	4120	U
49	5	4121	G
49	5	4124	G
49	5	4144	C
49	5	4163	U
49	5	4170	A
49	5	4183	G
49	5	4194	U
49	5	4195	G
49	5	4232	U
49	5	4254	G
49	5	4266	G
49	5	4291	G
49	5	4331	G
49	5	4348	A
49	5	4349	C
49	5	4375	C
49	5	4378	A
49	5	4379	A
49	5	4395	U
49	5	4448	G
49	5	4449	A
49	5	4453	C
49	5	4463	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	5	4475	G
49	5	4481	U
49	5	4488	A
49	5	4510	A
49	5	4512	U
49	5	4518	A
49	5	4519	C
49	5	4522	G
49	5	4527	G
49	5	4528	G
49	5	4548	A
49	5	4583	C
49	5	4589	A
49	5	4656	A
49	5	4670	C
49	5	4693	C
49	5	4699	U
49	5	4718	G
49	5	4719	G
49	5	4730	C
49	5	4752	U
49	5	4756	C
49	5	4770	U
49	5	4870	G
49	5	4872	G
49	5	4874	A
49	5	4885	U
49	5	4887	C
49	5	4888	U
49	5	4889	G
49	5	4900	C
49	5	4909	A
49	5	4910	G
49	5	4912	G
49	5	4926	C
49	5	4935	C
49	5	4945	G
49	5	4948	C
49	5	4950	U
49	5	4951	G
49	5	4965	U
49	5	4978	G

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Mol	Chain	Res	Type
49	5	4990	C
49	5	4991	U
49	5	5005	G
49	5	5016	A
49	5	5022	U
49	5	5026	U
49	5	5027	C
49	5	5041	G
49	5	5059	C
49	5	5060	A
49	5	5061	A
50	7	109	U
51	8	2	G
51	8	38	U
51	8	62	A
51	8	94	G
51	8	104	A
51	8	110	U
51	8	111	U
51	8	124	U
51	8	125	C

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	5MU	2	54	48	19,22,23	1.49	4 (21%)	28,32,35	1.98	8 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	5MU	2	54	48	-	2/7/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	2	54	5MU	C6-C5	3.34	1.40	1.34
48	2	54	5MU	C2-N1	3.13	1.43	1.38
48	2	54	5MU	C4-C5	2.69	1.49	1.44
48	2	54	5MU	C4-N3	-2.13	1.34	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	2	54	5MU	N3-C2-N1	4.82	121.28	114.89
48	2	54	5MU	C4-N3-C2	-4.22	121.89	127.35
48	2	54	5MU	C5-C4-N3	3.88	118.62	115.31
48	2	54	5MU	O4-C4-C5	-3.33	121.04	124.90
48	2	54	5MU	C5M-C5-C4	2.83	121.88	118.77
48	2	54	5MU	C6-N1-C2	-2.37	118.90	121.30
48	2	54	5MU	C3'-C2'-C1'	2.18	105.58	101.43
48	2	54	5MU	O2-C2-N3	-2.07	117.65	121.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	2	54	5MU	O4'-C4'-C5'-O5'
48	2	54	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 164 ligands modelled in this entry, 164 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
46	x	14
49	5	13
46	y	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	1211:UNK	C	1300:UNK	N	25.67
1	x	608:UNK	C	700:UNK	N	22.35
1	x	1014:UNK	C	1100:UNK	N	19.48
1	x	817:UNK	C	900:UNK	N	18.97
1	y	223:UNK	C	250:UNK	N	18.15
1	5	4776:G	O3'	4859:C	P	18.06
1	5	757:G	O3'	906:C	P	17.33
1	5	519:C	O3'	642:G	P	16.68
1	x	1318:UNK	C	1400:UNK	N	16.67
1	5	2910:G	O3'	3583:U	P	16.41
1	5	2131:C	O3'	2243:C	P	14.71
1	5	3950:U	O3'	4065:G	P	14.58
1	y	116:UNK	C	150:UNK	N	14.39
1	y	62:UNK	C	100:UNK	N	14.33
1	x	713:UNK	C	800:UNK	N	13.69
1	5	997:C	O3'	1047:C	P	13.50
1	y	15:UNK	C	50:UNK	N	13.30
1	y	465:UNK	C	500:UNK	N	13.06
1	y	171:UNK	C	200:UNK	N	12.23

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	515:UNK	C	600:UNK	N	11.79
1	y	413:UNK	C	450:UNK	N	10.77
1	y	309:UNK	C	350:UNK	N	10.39
1	x	55:UNK	C	100:UNK	N	9.70
1	5	1051:G	O3'	1064:G	P	9.28
1	y	516:UNK	C	550:UNK	N	9.23
1	x	926:UNK	C	1000:UNK	N	8.71
1	y	266:UNK	C	300:UNK	N	8.32
1	x	111:UNK	C	200:UNK	N	6.50
1	x	1118:UNK	C	1200:UNK	N	6.08
1	x	409:UNK	C	500:UNK	N	6.02
1	x	216:UNK	C	300:UNK	N	5.93
1	x	309:UNK	C	400:UNK	N	5.87
1	5	1222:A	O3'	1232:G	P	4.65
1	y	367:UNK	C	400:UNK	N	4.13
1	5	1699:A	O3'	1718:C	P	3.82
1	5	1100:U	O3'	1167:C	P	3.77
1	y	564:UNK	C	600:UNK	N	3.18
1	5	4942:C	O3'	4944:C	P	2.75
1	5	4939:C	O3'	4941:G	P	2.65

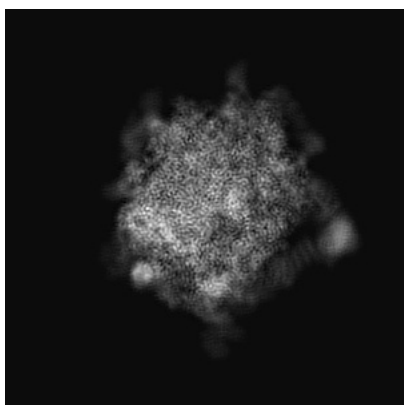
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2832. These allow visual inspection of the internal detail of the map and identification of artifacts.

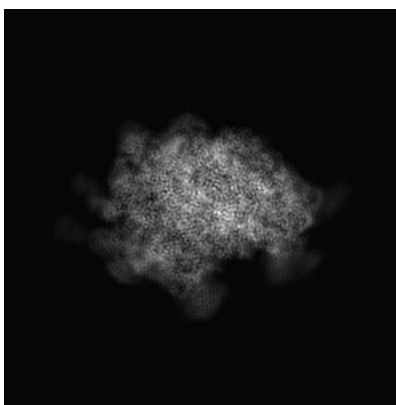
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

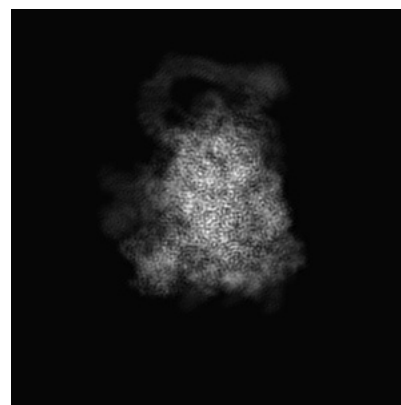
#### 6.1.1 Primary map



X



Y

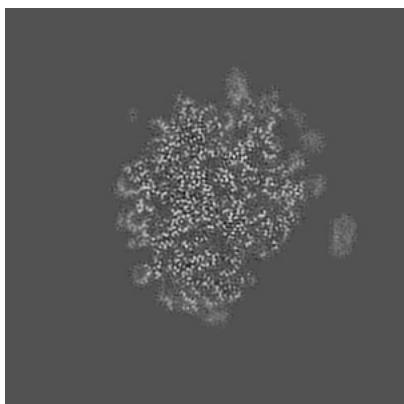


Z

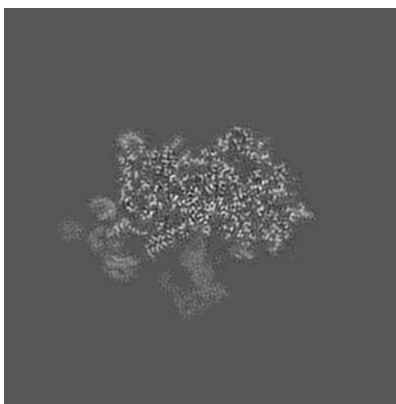
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

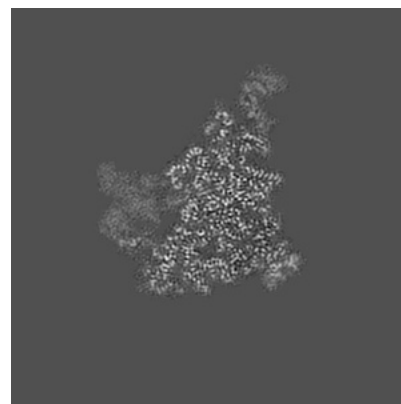
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

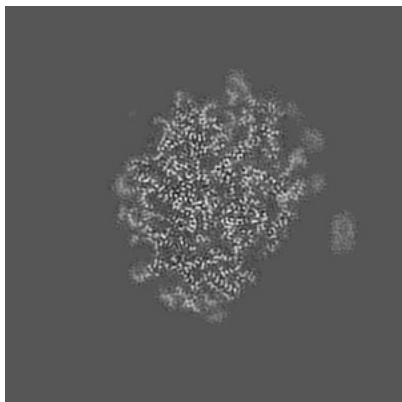


Z Index: 160

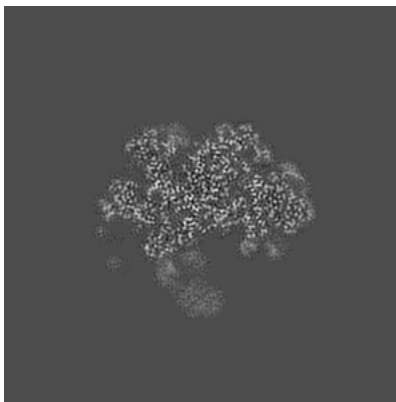
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

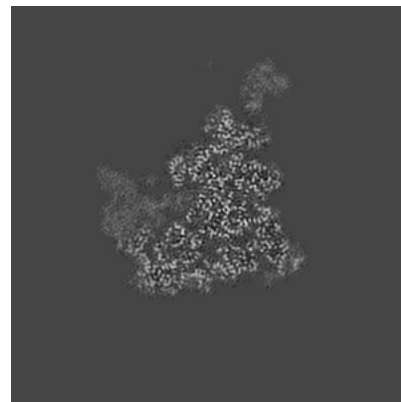
### 6.3.1 Primary map



X Index: 158



Y Index: 149



Z Index: 156

The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

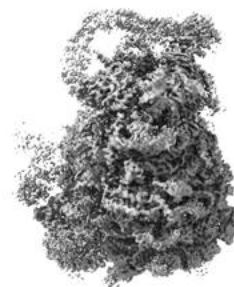
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

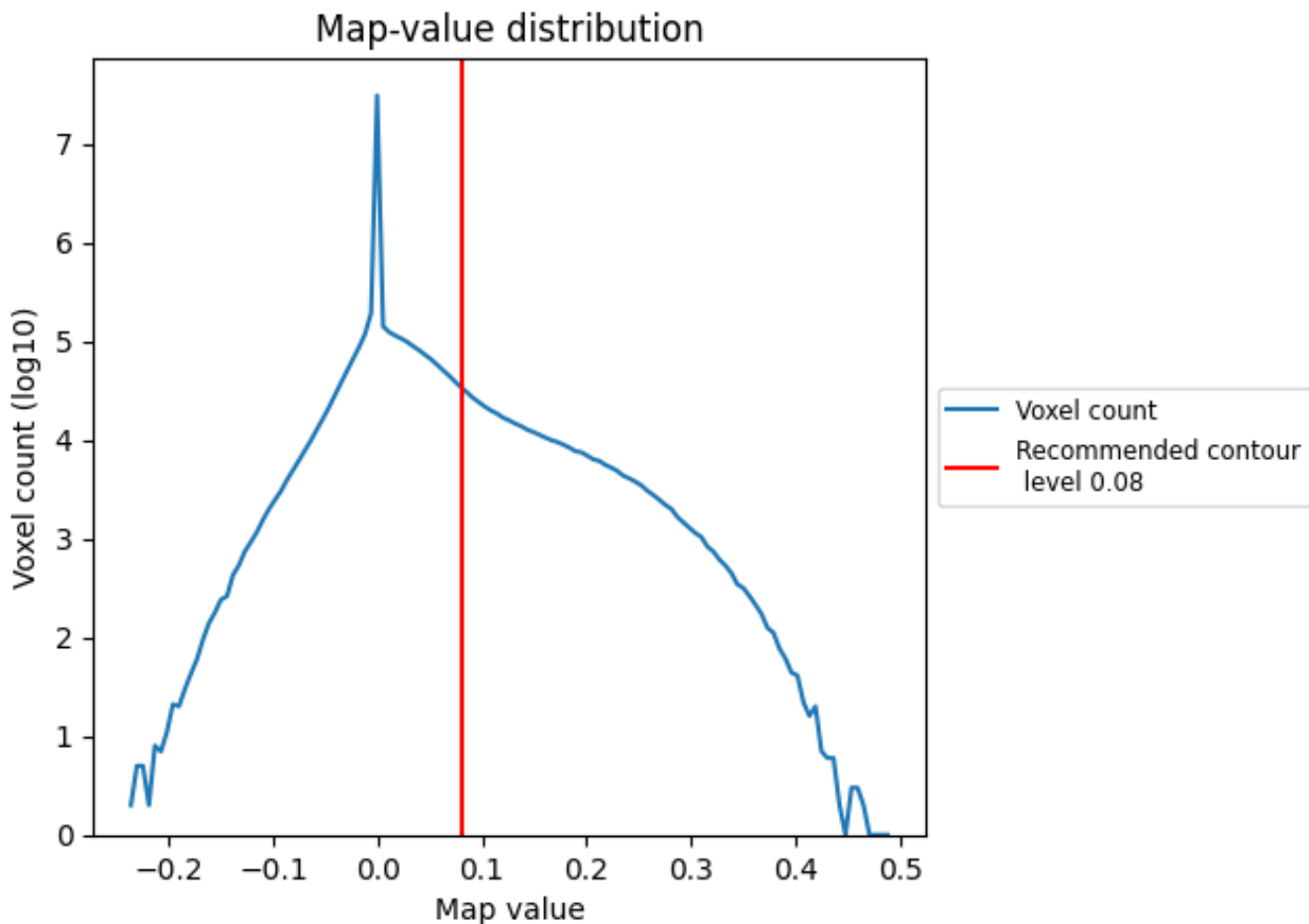
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

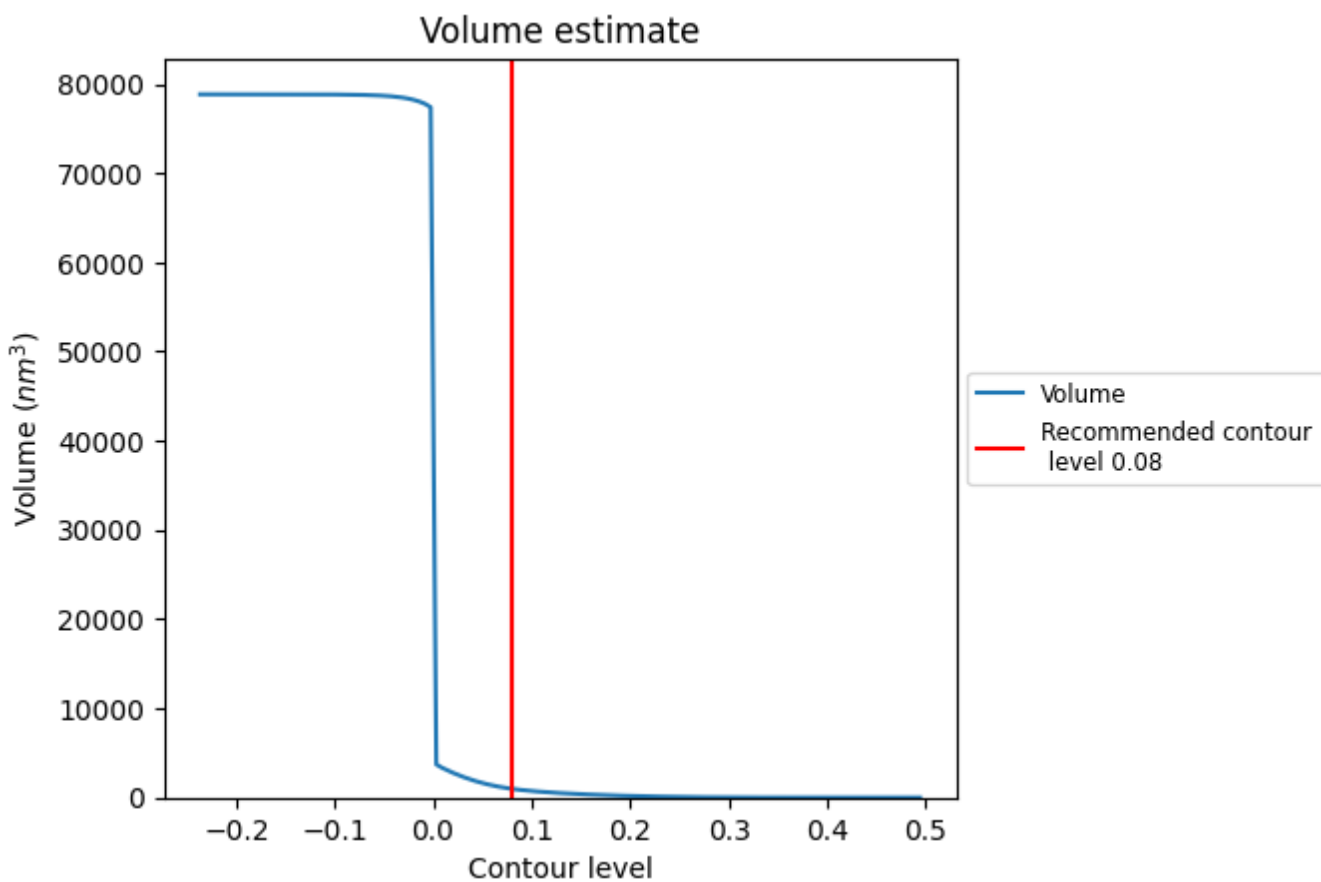
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

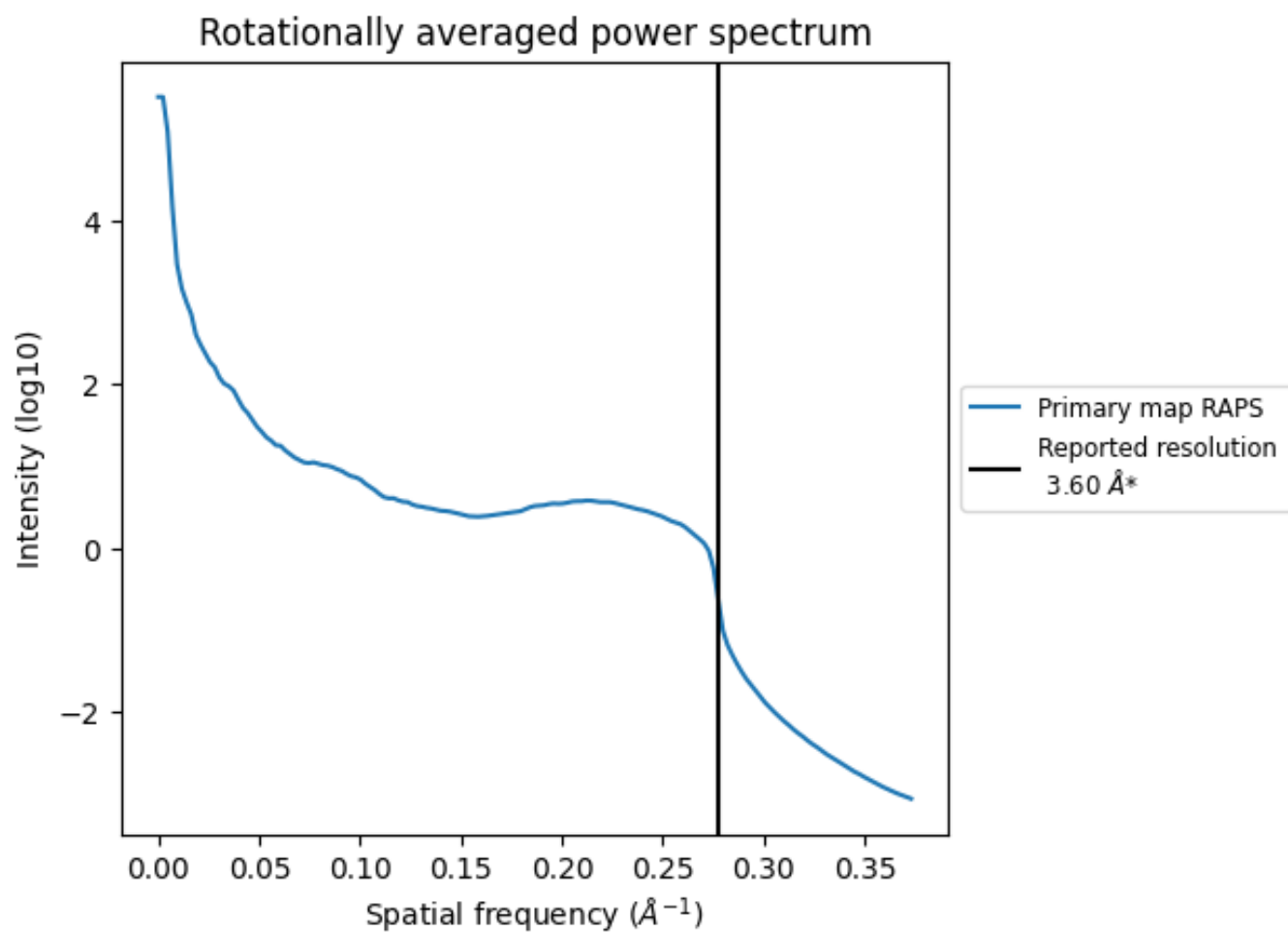
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 982 nm<sup>3</sup>; this corresponds to an approximate mass of 887 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.278 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation

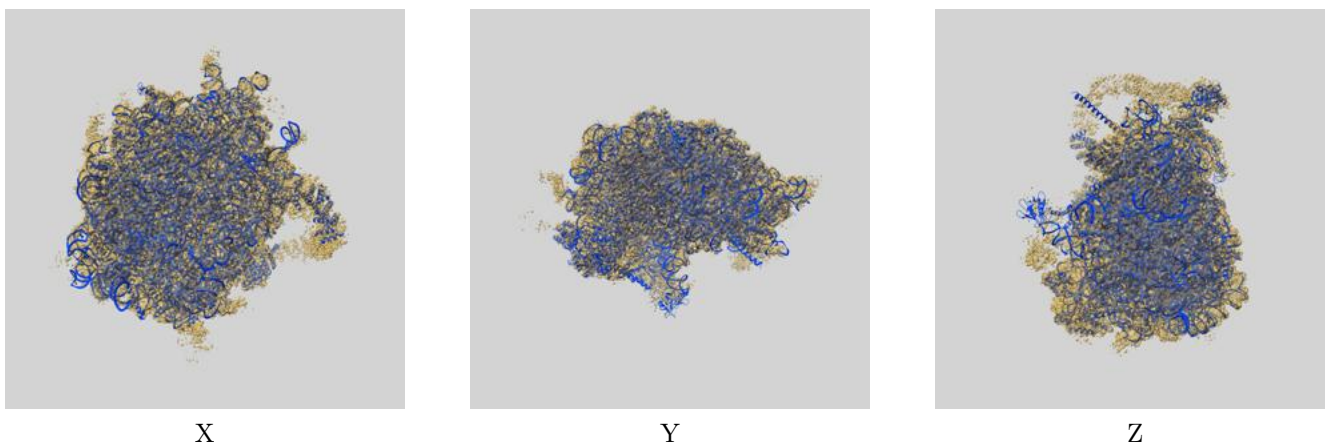
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

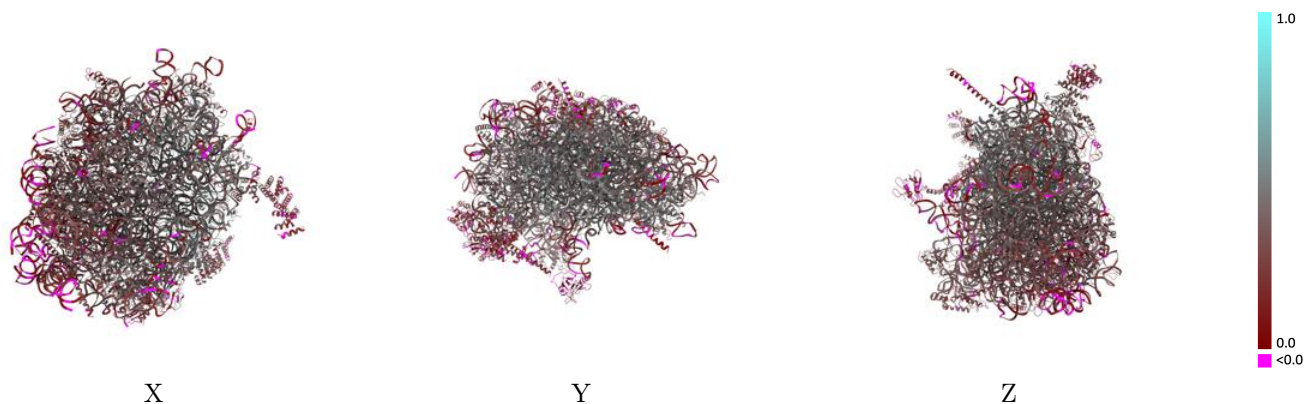
This section contains information regarding the fit between EMDB map EMD-2832 and PDB model 3J92. Per-residue inclusion information can be found in section 3 on page 14.

### 9.1 Map-model overlay [i](#)



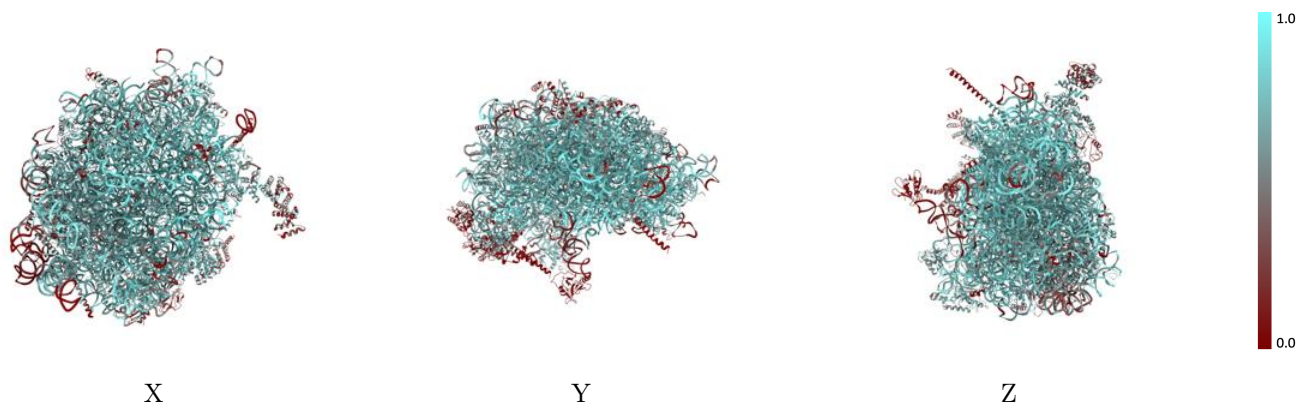
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [\(i\)](#)



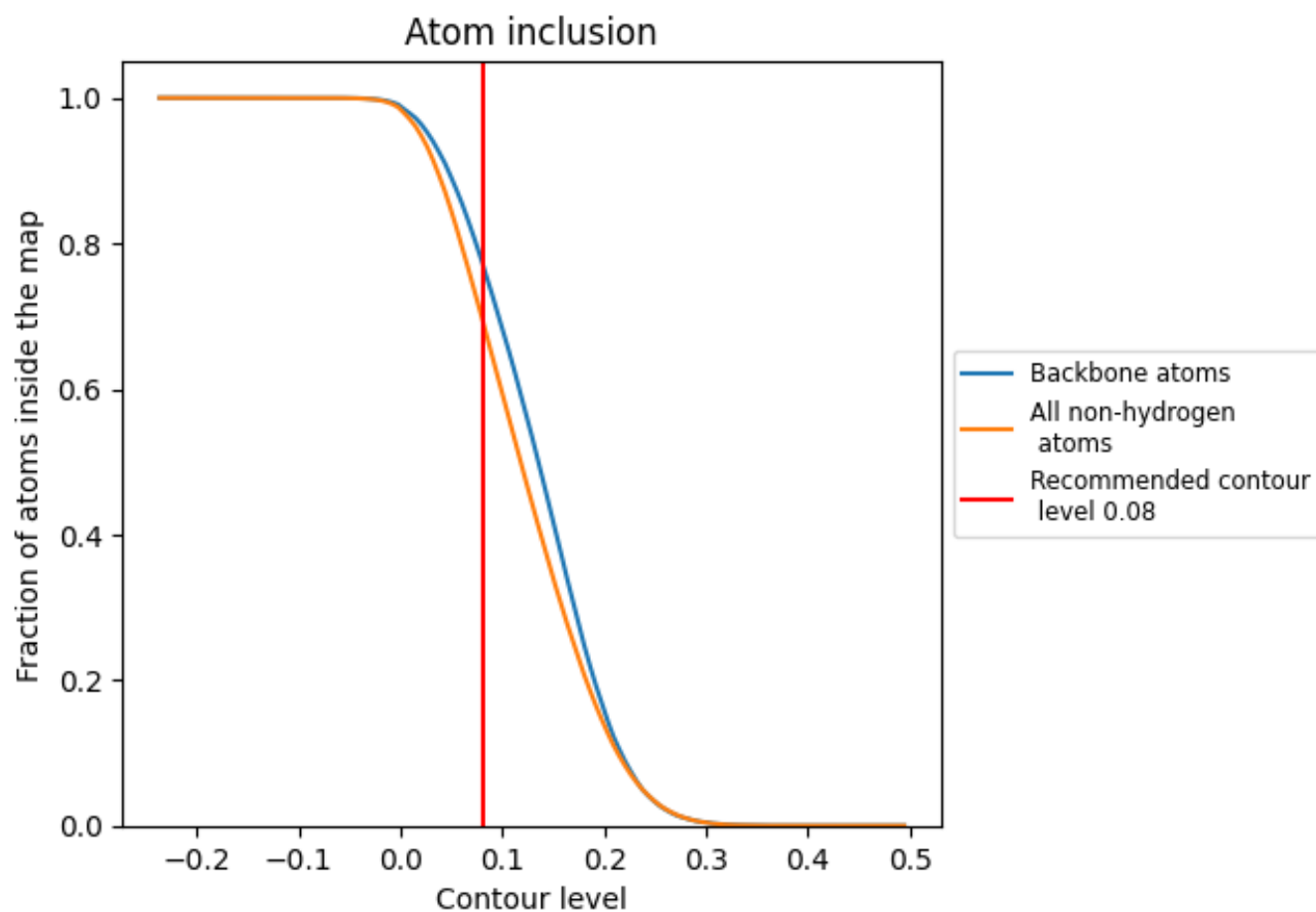
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary











































The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6966	 0.3400
0	 0.1045	 0.1200
1	 0.4959	 0.3720
2	 0.1424	 0.1480
5	 0.7507	 0.3290
7	 0.7885	 0.3270
8	 0.7774	 0.3580
A	 0.7643	 0.4550
B	 0.7693	 0.4700
C	 0.6623	 0.3490
D	 0.6232	 0.2770
E	 0.6089	 0.3340
F	 0.6591	 0.3210
G	 0.5915	 0.3360
H	 0.6804	 0.3990
I	 0.6843	 0.3810
J	 0.6240	 0.3070
L	 0.6224	 0.3110
M	 0.6946	 0.3750
N	 0.7327	 0.3860
O	 0.7359	 0.4310
P	 0.7531	 0.4430
Q	 0.6542	 0.3320
R	 0.6343	 0.3880
S	 0.6957	 0.3580
T	 0.6469	 0.3510
U	 0.6785	 0.4340
V	 0.7526	 0.4820
W	 0.7112	 0.4620
X	 0.6828	 0.4060
Y	 0.6809	 0.3670
Z	 0.6887	 0.4210
a	 0.6953	 0.3540
b	 0.5505	 0.2830
c	 0.7259	 0.4490



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Chain	Atom inclusion	Q-score
d	 0.7001	 0.4590
e	 0.7050	 0.3930
f	 0.7387	 0.4080
g	 0.7084	 0.4350
h	 0.6487	 0.3590
i	 0.6391	 0.3470
j	 0.7493	 0.4210
k	 0.5799	 0.3760
l	 0.7021	 0.4410
m	 0.7091	 0.4040
o	 0.6477	 0.3570
p	 0.7184	 0.4660
r	 0.6774	 0.3480
s	 0.2367	 0.1680
t	 0.2130	 0.1390
u	 0.0109	 0.0690
v	 0.3544	 0.2610
w	 0.4906	 0.3660
x	 0.4688	 0.2410
y	 0.4038	 0.2100
z	 0.4927	 0.3510